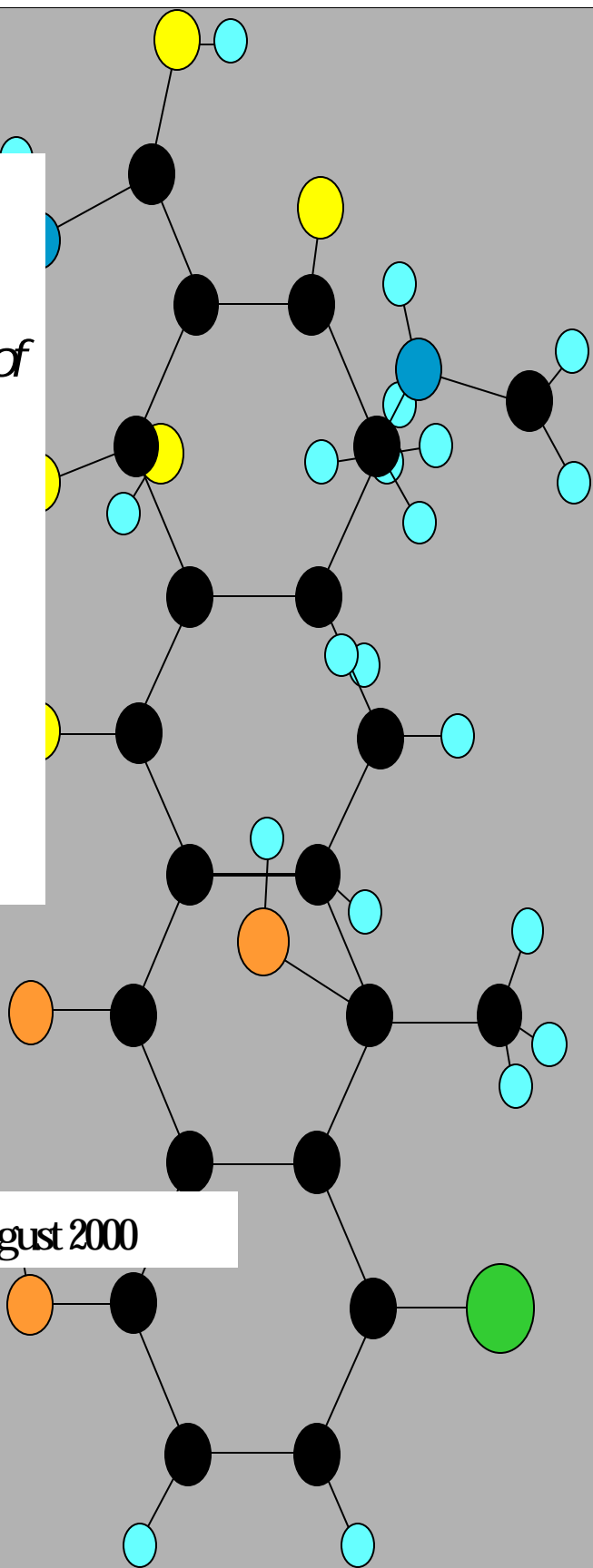


*Vision 2020
Chemical Industry of
The Future*

**Technology
Roadmap for
Materials**

August 2000



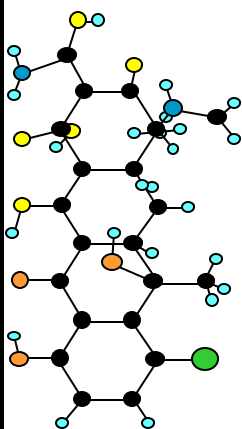


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Executive Summary

The chemical industry has prepared a vision of how it will meet its competitive challenges through the year 2020{*Technology Vision 2020: The Chemical Industry*, available from the American Chemical Society, <http://www.acs.org>}. To put this vision into a working format, a number of technology workshops in areas defined as crucial to the progress of the chemical industry are being conducted.

This technology roadmap addresses the materials technology subset of new chemical science and engineering technology, a key area of research in *Vision 2020*. It was developed with the support and guidance of the **Vision 2020 Materials Technology Committee**, a group comprised of key individuals from industry, government and academic institutions. To gain input for the roadmap, two workshops were held to cover five major topic areas: 1) New Materials, 2) Materials Characterization, 3) Materials Modeling and Prediction, 4) Additives, and 5) Disassembly, Recovery, and Recycle.

The primary objective of the materials technology committee and these workshops was to define actionable recommendations for future research projects involving industry, academic laboratories and government agencies which can have a significant impact on the future of the domestic chemical (materials) industry. The key research objectives identified are summarized below.

New Materials

- **Explore New Concepts in Catalysis for Polymers.** Catalysis is viewed as the technology area that has been the driving force behind major advances in new polymers over the past several decades. It is recognized that a lot of technology and fundamental understanding remains undeveloped leaving significant opportunities for long range concerted research. Related ideas include: 1) C1 chemistry applied to monomers, 2) ethylene (and polar functional monomers in polymers), and 3) new materials from alternate processes (e.g., using monomers not used today, under different conditions).

The improved predictability/design of catalyst structure/activity would have a major impact on the development of new polymers and optimization/improvement of existing polymers. The ability to combine low cost monomers into new materials depends primarily on new catalyst technology. While there is a renaissance in transition metal catalysis for polymerization, the technology is still largely empirical. A need exists to develop predictive techniques (computational modeling) to allow more rational design of new catalysts. Combinatorial methodology would also fit this area (and has been noted in another **Vision 2020** roadmap).

- **Study of Polymer-Structure Property Relationships.** Although this is a very broad topic, certain areas have been clearly suggested which fit this theme. A key area involves the development of technology (models) to predict lifetimes of polymers and degradation failure. This emerged as a priority area in both workshops on New Materials.
- **Colloid/Interfacial Science.** This broad area includes extending new concepts in colloid science to polymers, extending concepts from ceramic science to polymers, creation of novel nanoporous, nanoscale structures, understanding surfactant fundamentals, and understanding

thin film adhesion. The need for understanding of surface chemistry of additives and interfacial reactions was identified here and in the additives area.

- **Continued Development of Composite Technology for Non-Military Applications.**

While the end of the cold war reduced the polymer-based composite development that was primarily driven by military support, a renewal of interest in composites for non-military applications appears to be emerging. This would include transportation infrastructure and fabrication, structural adhesives and architectural applications. Areas noted for composites research include characterization of composites during fabrication, adhesion for structural applications and interfacial reactions between polymers and diverse materials.

- **Continued Development of New Materials.** Another category which expectedly emerges is novel materials. No specific area came as a clear priority, however, several important areas need to be noted: controlled (living) free radical polymerization, organic-inorganic composites and new monomers. The significant markets for polymers in emerging electronic/optoelectronic markets is well-recognized but not specifically discussed in this roadmap as other roadmaps exist (e.g., Sematech).

Materials Characterization

- **R&D Tools.** New techniques for composition, structure, and dynamics for buried interfaces are critical to advances in materials characterization. Imaging techniques (3-D, chemical information imaging, mechanical imaging) and high through-put assay methods for generation of databases are a top priority.
- **Real-Time Measurements.** Development of on-line, spatially resolved, non-contact measurement techniques are important for both materials processing and new materials development. Non-invasive control devices that are embedded in a material on the molecular level could completely change the nature of today's materials and how they are manufactured.

Materials Modeling and Prediction

- **Methods Development.** In the near term, the need to develop accurate potentials and methods at mesoscale dimensions is considered a high priority. In the longer (on-going) time frame, the need for a multi-disciplinary, coordinated theory/modeling/experimental research effort in interfaces is considered high priority. Key areas include: 1) colloid science/interfacial science (new materials), 2) biomaterials and biotechnology (new materials), 3) additives: need for understanding surface chemistry, and 4) catalysis: need for better modeling tools and concerted efforts.
- **Theory.** A critical need in modeling theory is improved bridging techniques, including research on renormalization group approaches, mapping and reverse mapping, and bridging length and time scale. The need to develop better theories and modeling methodology for non-equilibrium meshes with the need for improved prediction of polymers aging/life time. A need exists to develop basic theory for materials science as a short term goal.

Additives

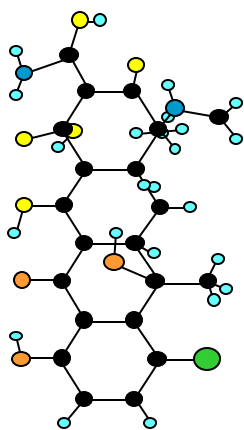
- **Prediction/Modeling.** The need for a multi-scale portfolio of computational methods for additives and the effect on polymers is a high priority.
- **Interfacial Methods/Fundamentals Applied to Additives.** The need to understand surface chemistry/ interfacial interactions of additives is a priority topic and meshes with a similar need noted in the new materials sessions.
- **Nanoparticles.** This area emerged in enough recommendations to be combined into a priority subject. The need for high surface area fillers to enhance the properties of polymers appears to be an area where significant performance benefits could be realized. Nanoparticle inorganics could offer reinforcement benefits not realized by their micron-sized analogies. Particle reinforcement at the nanoscale exist with carbon black and glass (cab-o-sil) but not for the myriad of other inorganic materials. Development of processes to produce nano-particles from the available inorganic fillers could lead to enhanced performance and the development of a new class of materials.

Disassembly, Recovery and Recycle

- **Collection of Raw Materials.** Two key areas are the development of efficient sorting technology and incentives to motivate end-users to send materials into the recovery stream.
- **Deriving Pure Monomers and Intermediates From Polymers.** A high priority is to develop technology to isolate pure monomers from mixed polymers. A closely related priority is developing the capability to depolymerize at low temperature and pressure (including thermosets).
- **Chemistry for Mixed Polymers Streams and Polymers Modification.** Chemistry is needed to improve the properties of composites, synthetics, and bio-based materials and to develop functional polymers to facilitate recyclability. Compatible chemistries and processes for mixed polymers is also a high priority. Technologies are needed to restore the performance of contaminated polymers, and to remove contaminants.
- **High Yield Separation Processes.** The highest priority identified is the development of technology and processes to separate equivalent-density polymers. Sorting and separating polymers flakes, including methods to quickly identify the polymers in a sample of mixed polymers flakes, is another high priority.

Other

An overlapping theme from many of the workshop subjects involved interfacing material sciences with life sciences. As many of the larger chemical companies are embarking on large biotechnology research projects, the overlap of the disciplines is even more important. These distinct technology areas often approach, analyze and solve problems employing different methodologies. In essence, they do not “speak the same technical language.” An interdisciplinary approach involving materials science with life science to investigate areas of mutual interest will be necessary to solve future needs in both areas. Government sponsored interdisciplinary programs at the interface between these technical areas should be encouraged.



1 Overview

The Challenges Ahead

The chemical industry faces considerable economic, environmental and societal challenges during the 21st century. Major forces for change include the increased globalization of markets; societal demand for improved environmental performance; the need for increased profitability and capital productivity; higher customer expectations; and changing work force requirements.

The chemical industry has outlined a vision of how it will meet its competitive challenges through the year 2020 in *Technology Vision 2020: The Chemical Industry*.¹ *Technology Vision 2020* is the chemical industry's response to a White House Office of Science and Technology Policy request for industry advice on improving the allocation of government R&D funding to advance the manufacturing capability and competitiveness of U.S. industry. One of the important conclusions of *Vision 2020* was that the growth and competitive advantage of the chemical industry would depend upon the collaborative efforts of industry, government and academia.

A key element in meeting future challenges is technology research, development and deployment. As part of its strategy for achieving future goals, the chemical industry is developing technology roadmaps in several crucial areas. Technology roadmaps link the strategic goals outlined in *Vision 2020* with a detailed research agenda of near-, mid- and long-term technology R&D. Through technology roadmaps, the industry hopes to provide a way for decision-makers to make strategically-driven investments in R&D that will increase profitability while achieving goals for improved energy efficiency, safety, and environmental performance.

The Role of Materials Technology

Materials technology is one of the many areas targeted by the chemical industry for technology roadmapping activities. Materials play a critical role in the economic performance and growth of the chemical process industries, and new materials technology will be an essential part of the industry's strategy for achieving its vision. Materials are an integral and important component of the chemical industry. Materials contribute a large amount to industry revenues, and represent a

¹

Available from the American Chemical Society, Washington, D.C., (202) 452-8917.

high growth portion of the industry. Annual trade in polymers, engineered polymers and fibers amounts to about \$275 billion every year.² The development of new materials and materials technology have been identified as a priority research area in nearly all chemical industry roadmap activities to date. Among these are technology roadmaps for separation processes, new process chemistry, biocatalysis, materials of construction, and others.

Advances in materials technology are discussed throughout *Technology Vision 2020* as important industry needs and challenges. Many of these advances directly relate to the development of new materials, improving the performance of existing materials, and improving the processes used to manufacture materials. Figure 1-1 illustrates the needs and challenges for materials technology that are identified in the chemical industry's vision for the future. Many of these are addressed in this technology roadmap, particularly those shown under the materials technology and chemical measurement categories.

The **Materials Technology Vision 2020 Committee** was assembled in the spring of 1998 to lead the development of a roadmap for materials technology to respond to *Technology Vision 2020*. The Committee is comprised of the following members from industry, government and academic institutions:

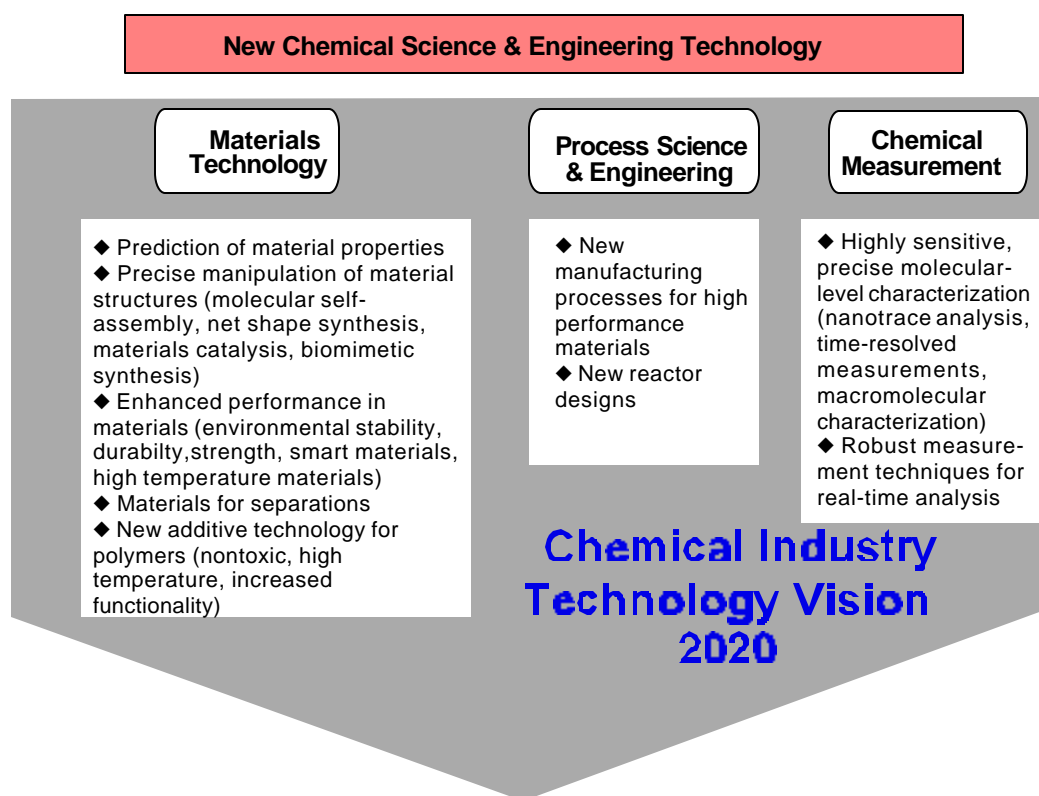


Figure 1-1. Materials Needs and Challenges in *Vision 2020*

²

Society for the Plastics Industry. *Year End Statistics for 1998, Production Sales & Captive Use*.

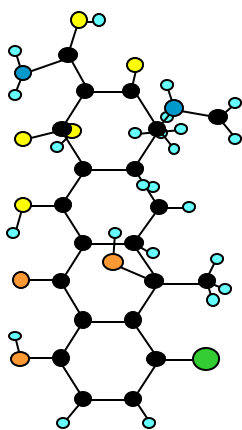
Chairman	Lloyd M. Robeson	Air Products and Chemicals, Inc.
Co-Chair	James E. McGrath	Virginia Polytechnic Institute and State University
	Don McLemore	Raychem, Inc.
	Don R. Paul	University of Texas
	Matt Tirrell	University of Minnesota
	Leslie Smith	National Institute of Standards and Technology
	Dave Moll	Dow Chemical Company
	Charles Sorrell	Department of Energy

Two technology roadmap workshops have been held to define material technology needs for the chemical industry. The first was held in November 1998, at University of Maryland University College in College Park, Maryland. The second was held in Golden, Colorado in September 1999. Summary reports are available for both workshops. The topics covered by these workshops included:

- **New Materials (covered in both workshops)**
Coordinators - Alan J. Lesser, Polymer Science and Engineering, University of Massachusetts, and Maria Spinu and R. Ritchie, DuPont
- **Materials Characterization**
Coordinator - Eric J. Amis, National Institute of Standards and Technology
- **Materials Prediction and Modeling**
Coordinator - Sharon Glotzer, National Institute of Standards and Technology
- **Additives**
Coordinator - Rick King, CIBA-Geigy
- **Disassembly, Recovery, and Recycling Technology**
Coordinator: Stephen S. Kelley, National Renewable Energy Laboratory

Sponsorship for the workshops was provided by the Council for Chemical Research, National Science Foundation, National Institute of Standards and Technology, and the U.S. Department of Energy. The focus of these workshops was on materials produced by the chemical industry with primary emphasis on polymers and their precursors. Ceramics and inorganic polymers were included if they constituted segments of the chemical industry. Metals, steel, concrete, and wood are materials covered in other industry segments and were not considered.

The results of both workshops form the basis for this technology roadmap. It provides a comprehensive research agenda that can be pursued by industry, academia, and government to guide future research partnerships and funding decisions. The R&D identified for materials technology will be critical to achieving the *Technology Vision 2020* goals to maintain and expand the U.S. chemical industry. It is a dynamic document, and will be reevaluated periodically to incorporate new market and technical information and to ensure that the research priorities remain relevant to the needs of both the chemical industry and its customers.



2 New Materials

Current Situation

The development of new materials has helped to fuel the growth of the chemical industry and has greatly impacted our quality of life during the last hundred years. Synthetic materials have been developed in some cases to take the place of traditional materials such as wood, glass, metals, and natural fibers. These new materials often perform better and provide increased flexibility in design and manufacturing.

Advances in composite materials (e.g., mixtures of polymers and fibers, of metals and ceramics) have greatly extended the range of performance and potential applications for these new materials. Blends of polymers and other materials have resulted in materials with better performance than single-polymer systems. The development of “smart” materials (e.g., electrochromics, controlled-release devices, shape memory alloys) allows materials to self-repair, actuate and transduce. New coating technologies, films, self-assembly or reactive approaches are under development to create materials with improved performance and unique properties.

The cost of developing and incorporating advanced materials is high. The reliability of new materials is unproven, and exploring their use is risky. Significant R&D, from bench scale experiments to the construction and testing of prototypes, is usually necessary before a new material can be implemented. Fabricability into cost-effective forms is often a significant barrier to the use of newly developed materials. In many cases, the expense and risk attached to new materials R&D puts it low on the corporate research priority list.

In spite of the risk, research into new materials is pursued by a number of companies, primarily for specific product applications. In the Federal sector, the U.S. Department of Defense supports a relatively large materials research program primarily focused on defense applications, although much of this research could be applied to industrial applications. The U.S. Department of Energy supports a diverse materials research program (Office of Energy Research, Office of Fossil Energy, and Office of Energy Efficiency and Renewable Energy/Office of Industrial Technologies) through universities, industry research institutes, and the national laboratories (Oak Ridge National Laboratory, Los Alamos National Laboratory, Sandia National Laboratory, and others). The research supported by the U.S. Department of Energy emphasizes the development of innovative new materials that improve the energy efficiency and environmental performance of industrial processes.

Goals for 2020: New Materials

A number of broad goals have been identified for new materials (see Figure 2-1). An important goal is to directly impact U.S. energy use through increased replacement of more energy-intensive materials (glass, paper, metals) with polymers. For processing efficiency, the goal is to produce large volume polymers using revolutionary new processes that are more cost-effective, energy efficient, and environmentally sound. A number of goals are related to developing new materials from biobased or novel feedstocks to displace conventional materials and create new material markets. An important economic goal is to maintain U.S. chemical industry world leadership through markets created by new materials. Goals for improving the effectiveness of research include expanding information on structures to the point where polymer design is made easier. This could be accomplished using libraries generated through combinatorial methods. Another goal is to maintain the level of R&D effectiveness over the next 20 years by ensuring that “discovery” R&D continues, i.e., research to enable breakthroughs in materials science. Such fundamental R&D efforts are critical if advances in materials technology are to be achieved.

Figure 2-1. Broad Goals for 2020: New Materials

Energy and Processing Efficiency

Achieve 20% energy savings by developing environmentally sound (from cradle-to-grave) polymers and polymer composites to replace more energy-intensive materials (glass, paper, metals)

- Produce commodity polymers using cost-effective, energy-efficient, environmentally benign, revolutionary new processes
 - S less expensive routes to monomers for condensation polymerization (e.g., gas - phase polymerization for EPDM rather than liquid phase)
 - S novel, less expensive means of polymerization
- Achieve integrated polymer design/processing for manufacturing
- Develop key enabling materials technology for alternative energy systems (proton exchange membranes, batteries, fuel cells) to allow a 25% reduction in fuel use

Economics

- Maintain U.S. chemical processing industry leadership in world markets through new materials
- Achieve 10% of revenues from new materials resulting from U.S.-based technology
- Displace conventional structural materials with polymer-based materials that are “materials of choice” (e.g., polymers with metal properties while retaining ease of processing and fabrication); achieve greater use of polymers in infrastructure applications (e.g. bridges).
- Create 10% of new polymers from sources other than petroleum (C1 chemistry, biomass, minerals, inorganics) through new/improved catalysts
- Identify and anticipate new markets for polymers

R&D Productivity

- Expand quantitative structure activity relationships (Q-SARS) to facilitate the design of polymers
- Maintain level of R&D effectiveness over next 20 years
- Reduce development cycle time and investment required to bring new materials to market

Opportunities and Applications for New Materials

Market Opportunities

New materials offer the promise of significantly expanding markets for the chemical industry (see Figure 2-2). The primary market opportunities where new materials could have an impact are in polymers and composites. Important applications include infrastructure, transportation/automotive components, medical/biological devices, electronic/optoelectronics, innovative textiles, light-weight power sources/energy storage and conversion, and structural adhesives. Light-weight power sources/energy storage and conversion, and polymers/composites for infrastructure (e.g., bridges and buildings) are relatively new areas for consideration. Polymeric materials used in electronic and optoelectronic applications could have a major impact

Figure 2-2. Market Opportunities for New Materials
(♦Priorities)

- Cost-competitive polymers and composites for:
 - S Transportation/automotive uses ♦♦♦♦♦♦
 - S Infrastructure ♦♦♦♦♦♦
 - S Hybrid materials, from structural nanomaterials to composites ♦♦♦♦♦
 - S Medical/biological (implants, living polymers, materials that interface with biological systems, drug delivery systems, transparent chemically resistant material) ♦♦♦♦♦
 - S Electronics/opto-electronics ♦♦♦
 - S Printed circuit boards (low absorption, cheaper, high T_g , low K)
 - S Ultra low dielectric electrical insulation and circuits ♦♦♦
 - S High-rise building construction ♦♦♦
 - S Enhanced oil recovery ♦
 - S Glass replacement for buildings and automobiles ♦
 - S Lower-pressure separations (water purification, wastewater treatment) ♦
 - S Electro-rheological applications (e.g., artificial hearts, automatic transmissions)
 - S Thermal insulation
 - S Light-weight, high-speed machinery
 - S Barrier materials (agricultural, packaging)
 - S Ballistic resistance
 - S Low-cost housing/sanitation
 - S Family housing/construction materials
 - S Space construction materials
- Better polymeric textiles (e.g., targets would be textiles comparable with natural fibers such as wool, cotton, silk and would be easily dyed and fabricated) ♦♦♦♦♦
- Light-weight power sources/energy storage and conversion ♦♦♦♦
- Adhesives to replace conventional metal fabrication techniques (e.g., structural adhesives to replace rivets) ♦♦♦
- High temperature proton exchange membranes ♦♦♦
- Organic materials with improved fire resistance ♦♦♦
- High volume applications such as thermopolymer elastomers (e.g., tires) ♦♦
- Low-cost, high-barrier packaging ♦♦
- Coatings (paint, scratch resistance, decorative, protective, higher performance, more environmentally benign)
- Coatings with zero emissions of volatiles
- Atmospheric carbon dioxide separation
- Aqueous high hardness glassy state coatings (rather than rubbery state at the end)
- Biodegradable polymers
- Photoelectric and electro-photic materials

considering the dramatic and continuing growth in these areas. Highly specialized applications include optical computing, materials with non-linear optical properties for optical switches, frequency modulation devices, and polymeric light-emitting diodes.

Technology Opportunities

There are many opportunities to develop enabling technologies that will foster the design and use of new materials (see Figure 2-3). A high impact area is the development of new catalysts for innovative materials. Unique composites and polymers with greatly improved properties may also be possible through advances in materials technology. These include polymer-based inorganic-organic hybrid materials, proton exchange membranes that are suitable for fuel cells, polymers that are intrinsically fire-resistant, water resistant polymers, polymers with controllable mechanical properties, and polymers that can withstand high temperatures. Entire new processing techniques are also possible, such as solid state processing or cold forging of polymers, and net shape polymerization.

Figure 2-3. Technology Opportunities for New Materials
(♦Priorities)

- New catalysts for novel materials (olefin monomer/comonomer) ♦♦♦♦
- Improved failure analysis for polymers ♦♦♦
- Polymer-based hybrids (organic-inorganic) ♦♦
- Proton-exchange membranes for fuel cells ♦♦
- Intrinsically fire-resistant polymers ♦♦
- Water-resistant/water borne polymers ♦
- Net-shape polymerization ♦
- High-temperature capability polymers ♦
- Polymer solvents for chemical processing ♦
- Bioprocesses to produce a source of monomers for polymers ♦
- Solid state processing/cold-forging of polymers ♦
- Polymers with small amounts of renewable, rather than made entirely from biomass ♦
- Processes that define material organization patterns, from submicron to macro scale ♦
- Polar monomer incorporation in olefin low-pressure processes ♦
- Polymers with controllable mechanical properties ♦
- Materials for more selective separations (robust membranes, catalytic membranes, dilute solutions, molecular level separations)
- Elastomers with better life cycle attributes
- Adhesives to marry
 - Polymers/polymers
 - Polymers/metals to replace welds
- Depolymerization catalysts/monomer recovery
- New property sets for existing monomers (synthesis and manipulation)
- Polymers with glass properties
- Optimized polymer-fiber interfaces
- Polymer-based nano-scopic structures
- Direct processes for moving from monomer to polymer (e.g., mold injected with catalyst and monomer)
- New thin film materials that can replace coatings
- Processes for ceramic-like materials
- Inexpensive polymers that are easily modified and fabricated by the user (like clay) and that can compete with wood and metal, eliminating expensive processing and fabrication methods
- Thermally reversible polymers that reassemble as they cool

Barriers to Development of New Materials

Modeling and Prediction

The highest-priority barrier for new materials is that adequate methodologies do not exist to predict the lifetime of polymers and degradation mechanisms. This data is readily available for competing materials such as steel and aluminum. A poor understanding of a material's performance over time may eliminate it from consideration in new products and equipment. The capability to predict catalyst structure/property activity and an understanding of structure/property relationships is essential for developing catalysts that will produce new polymeric materials. This knowledge is either not available or is very limited for many catalyst systems.

Fundamental Science and Chemistry

A critical barrier is the lack of entirely new cost-effective routes for manufacturing commodity polymers (polyethylene, polypropylene). Innovations in processing of these large volume polymers could have a substantial impact on the industry's competitive position in world markets. Another barrier the lack of effective catalysts for C1 compounds (having one carbon, such as carbon dioxide) which could serve as alternative feedstocks in producing new monomers. Catalytic chemistry and technology do not exist to make biological or living polymers, and are essential for further development of these unique materials.

Process Design/Development

The inability to match application needs with material property/process capabilities is a priority barrier for new materials development. Closely connected is the inability to control molecular structure during processing, which limits the ability to yield a material with accurately controlled properties. Process design limitations (e.g., thermodynamics, current solvents of use) also limit the development of many new polymers as well as advances in polymer production. There are significant processing issues associated with the use of C1-based polymers, such as overcoming the problem of activating the very stable carbon dioxide molecule.

Marketing/Economics

A significantly limiting factor in new materials development is that current development cycles are not cost-effective. This reflects the current inability to develop and market a product without excessive scale-up and marketing costs and time. New materials must have demonstrated performance before an industrial user/equipment manufacturer will consider their use in new applications. Another critical barrier is that targets for new materials development are not clearly defined, including identifying properties for specific applications. Meaningful metrics for R&D and value capture mechanisms are not available, making it difficult to justify investments and potential markets for new materials. High profit/high return opportunities are not being adequately identified and sold to upper level management, partly because of the inability to predict the performance of new materials until they are already in use (e.g., in the car, in the body). When coupled with the short-range outlook of most corporations and the desire to please stockholders, these barriers place significant constraints on new materials R&D.

Lack of risk-taking by management is a critical barrier for some high-risk development areas (e.g., medical materials) where liability and the potential for litigation increases the cost of development. These high costs limit exploration of many biomedical applications where the market volume is relatively small. Contributing to the problem is the fact that few tax incentives are available to promote new product development. Management is also reluctant to invest in creating an "entrepreneurial" influence in laboratories, particularly where returns are uncertain.

Regulations/Standards

A critical barrier is the function of the U.S. tort system and its impact on product liability. Diverting capital and operating investments toward compliance, environmental regulations and other standards may limit the amount of funds available for new material development (and exploratory R&D in general). Another issue is the lack of standards for polymeric materials, particularly performance-based standards, are not available, which makes it difficult for specifying engineers to include polymers as a materials selection choice in some applications.

Education

A significant barrier is the inadequate preparation of graduates with doctoral degrees for a position in materials development in industry. Today's required skills for new materials development are more diverse than just technical skills, and include a knowledge of marketing, entrepreneurship, polymer chemistry, fundamental science, and the ability to pursue team problem-solving.

Institutional Issues

The dissolution of long-range R&D laboratories creates a disconnect between industry and the basic sciences and represents a major barrier to advances in materials science. Overall, not enough government support is provided for the fundamental, discovery type of research needed to create technology breakthroughs. Many companies are not taking advantage of opportunities to work together on pre-competitive R&D that could benefit more than one firm. Another barrier is the poor understanding and interaction between scientific researchers and industry, which limits communication of industry's needs and ineffective direction of R&D.

High Priority Research Needs

Priority research needed to encourage the development of new materials is shown in Figures 2-4, 2-5 and 2-6. Research is organized by timeframe, i.e., when meaningful results and process improvements can be expected. A complete table of R&D needs is provided in Appendix B.

A successful approach to new material development will include require multi-disciplinary research teams; sustained efforts over time; new organizations such as joint industry, government and academic centers; more extensive use of undergraduate co-op mechanisms; the integration of polymer science into chemistry curricula; and a systems perspective for basic research.

Fundamental Science and Chemistry

Better understanding of intermolecular interaction is needed for design and control of structural function, and to enable greater control of super-molecular assemblies. Another high priority is research to understand the interfacial reactions between polymer and fiber, and polymers and metals. In this area the study of thin film adhesion and bonded interfaces (silicon, dispersed platinum-carbon) is a top priority. This research is essential for promoting the use of polymers in applications where they must function as mating parts with other materials. It will also improve understanding and development of effective joining techniques for polymers and other materials.

An on-going research effort in all aspects of colloid science is a top priority. An important element of this activity would include the extension of new colloids and colloid science to

**Figure 2-4. Priority R&D for New Materials:
Fundamental Science, Engineering and Polymer Chemistry**

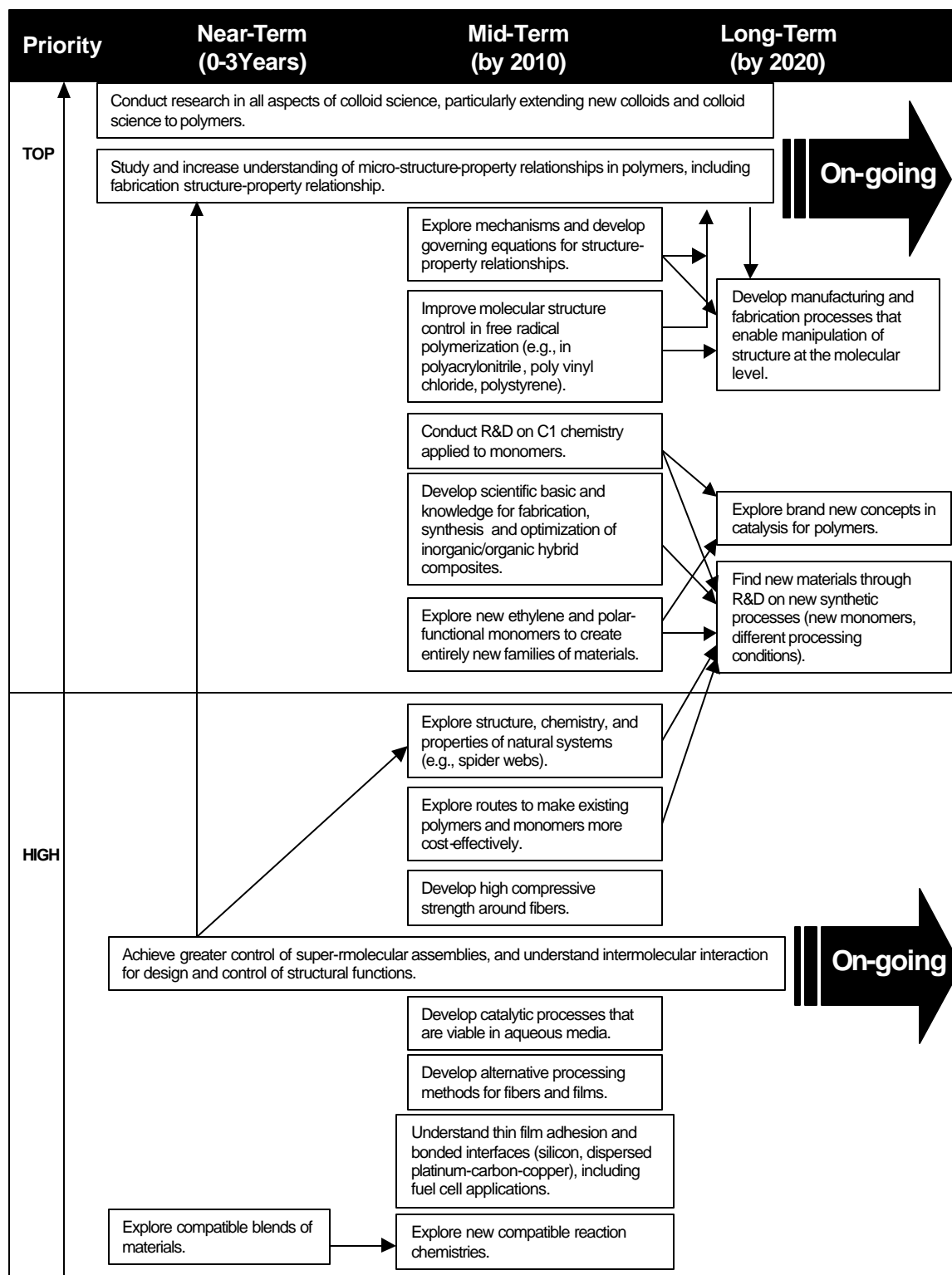


Figure 2-5. Priority R&D for New Materials: Specialty Materials

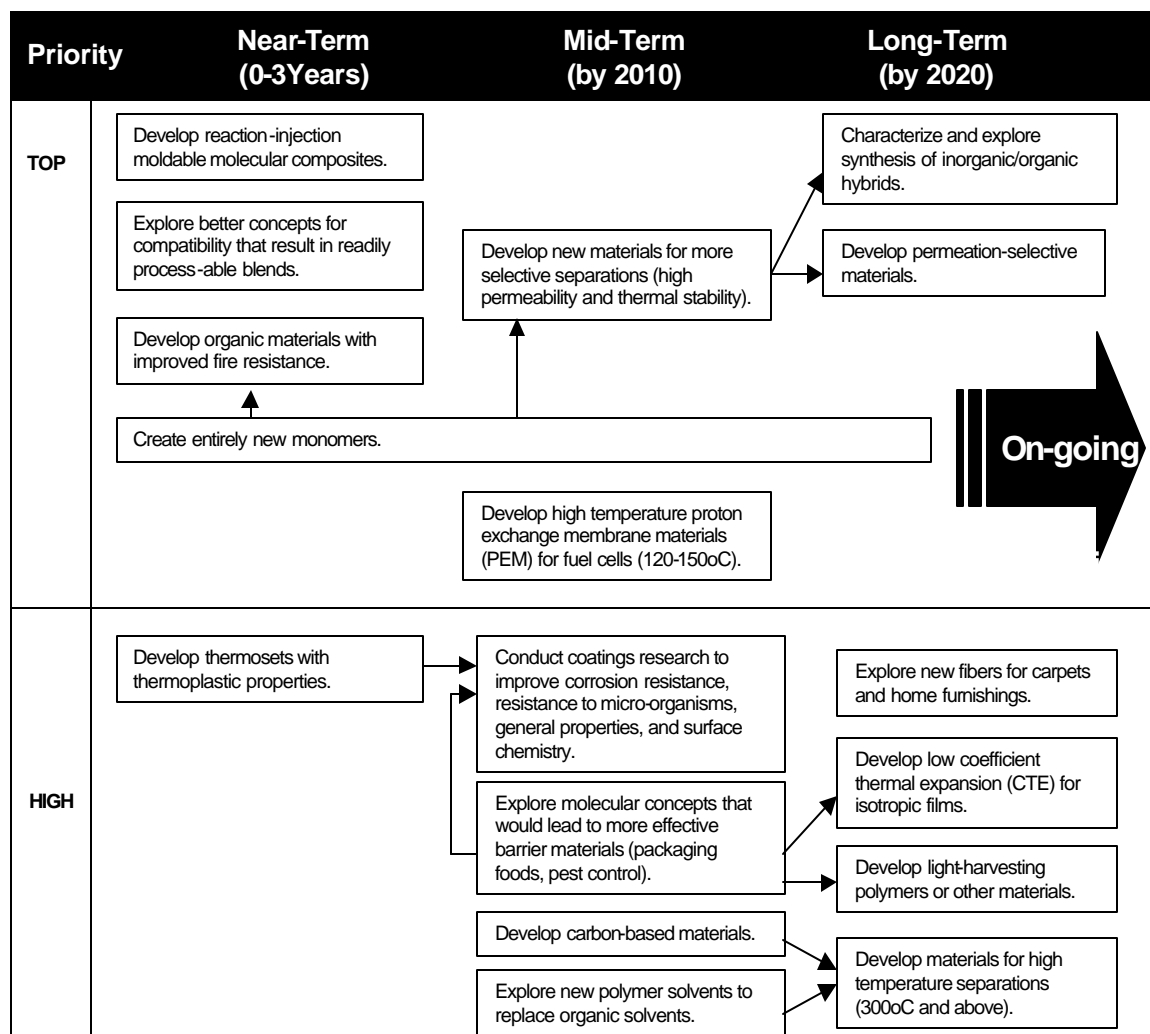
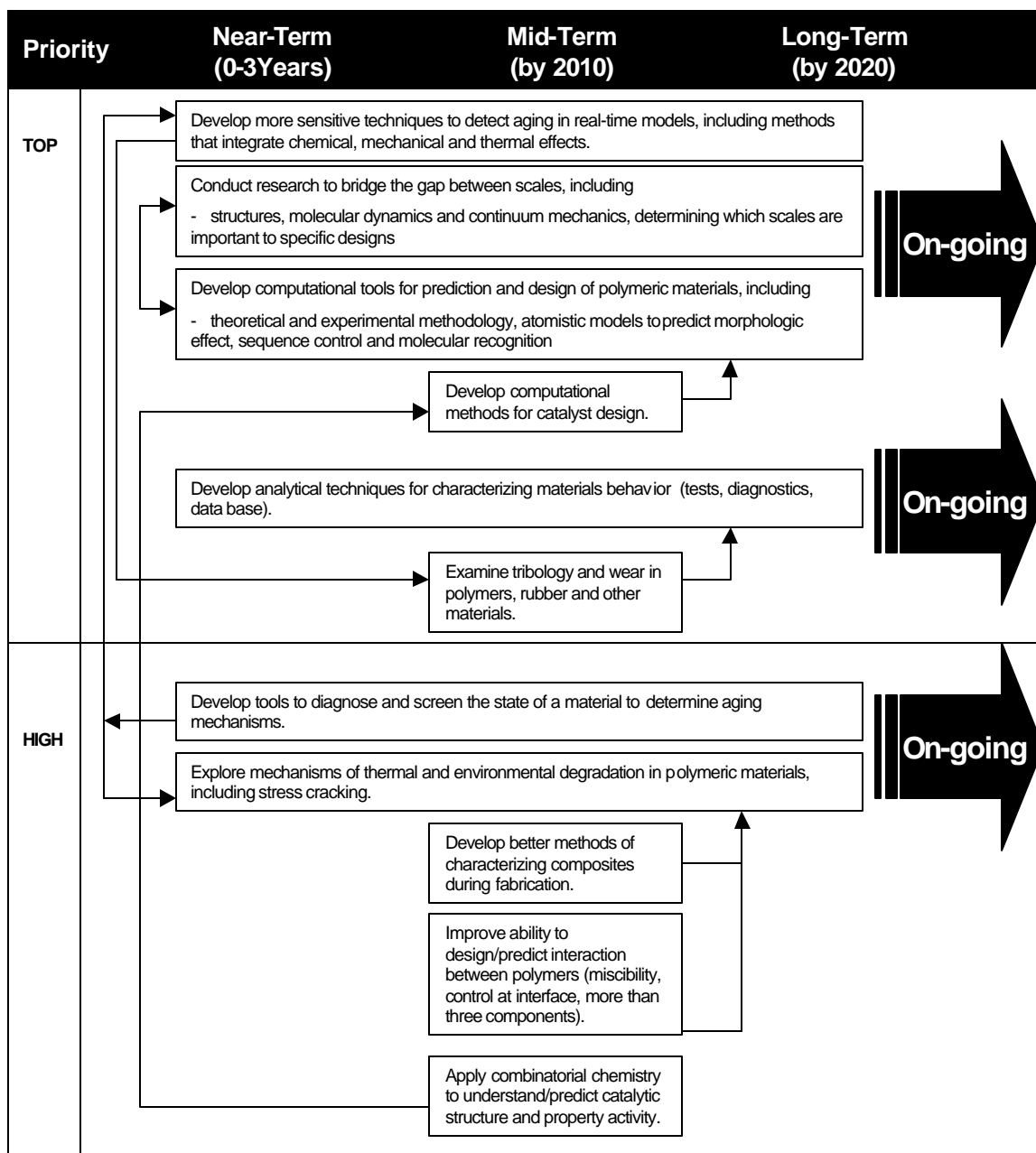


Figure 2-6. Priority R&D for New Materials: Prediction, Simulation, and Characterization



polymers. This area of science has experienced tremendous growth as a result of advances in ceramic science, and many new tools and scientific methods are now available that could be applied to polymers.

An understanding of the equations governing structure-property relationships is a priority need for new materials, including the ability to control molecular structure during free-radical polymerization. One component is understanding fabrication structure-property relationships at the microstructural level.

In the area of synthesis, the top priority is to apply C1 chemistry to the production of monomers, and explore these compounds as potential feedstocks. One area of interest is catalyst research related to carbon dioxide addition reactions. Another top priority is the exploration of completely new and innovative concepts in catalysis for polymers that are radically different from current practice. One possibility is to look at new ethylene and polar-functional monomers as potential precursors for entirely new families of polymers. Exploring entirely new synthetic processes (such as using monomers not currently used today, under different conditions) is a priority in the search for new materials. One potential approach is one-pot cross-linking technology at ambient conditions, which would require new cross-linking chemistry. This technology could enable coating systems based on customer requirements that would not need to be mixed before application.

Process Design/Engineering

Research is needed to explore manufacturing and fabrication processes that enable manipulation of polymer structure at molecular levels. Such processes would enable production of polymers with greater control of quality and performance. Alternative processing methods may be needed for the next generation of polymers (particularly films and fibers), along with appropriate process simulation models. These may include catalytic processes that work in aqueous media rather than some of the very toxic solvents now used for polymerization. New, viable bioprocesses are also needed to take advantage of biomass resources as a feedstock for producing monomers for new products. Overall, the objective is to improve materials processing conditions to use less energy, create fewer emissions, and lower temperatures and costs.

Specialty Materials

As a route to new materials, characterizing and exploring the synthesis of inorganic/organic hybrids is a high priority. These materials could be important in many industrial applications, particularly separations technology. Research is also needed to develop a scientific basis for fabrication and optimization of hybrid composites. Another high priority is to explore better concepts for compatibility that will yield readily processable polymer blends with higher performance and selected properties than are currently available.

Top priorities with large market potential are organic materials with improved fire resistance, and high temperature proton exchange membrane (PEM) materials for use in fuel cells operating at 120-150°C. Exploration of molecular concepts is needed to develop materials that can serve as more effective barriers for packaging foods and for pest control. Of particular interest would be barriers that prevent permeation of oxygen, carbon dioxide, and water. To fully expand markets, exploratory research is needed to develop new materials with desirable properties such as high permeation selectivity, high temperature capability (above 300°C), biodegradability, natural fiber-like properties, corrosion and microorganism-resistance (coatings), low coefficient of thermal expansion, and moldability.

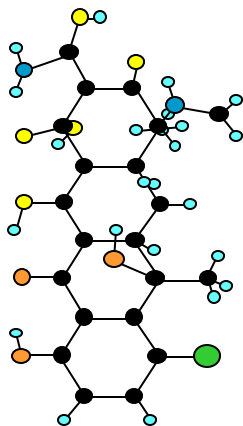
To enlarge the feedstock resource, research is needed to develop carbon-based materials and renewables as polymer building blocks. This includes investigation of entirely new monomers and their associated chemistries. An example is new chemistry and catalysts for conversion of biomass to condensation polymers.

Prediction, Simulation

The highest-priority research need is to understand the structure, molecular dynamics, and continuum mechanics between scales, including design specifications. Analytical techniques are needed for characterizing material behavior, particularly how composites perform during

fabrication processes. Computational tools are needed to predict the performance and property characteristics of polymers and catalysts. These tools will aid in the design of new polymeric materials as well as the catalysts needed to initiate polymerization reactions. Catalysis is an area where advances in prediction can have a major impact on the future polymer industry which increasingly relies on exotic catalysts for new and improved products from commercially available monomers. Overall, a priority is to use combinatorial technology and methods to design, produce and select polymers. This area is discussed in more detail in Chapter 4, Materials Modeling and Prediction.

The highest priority in lifetime prediction is the development of more sensitive techniques to detect aging in real-time. Ideally, methods would combine chemical, mechanical, and thermal effects to evaluate aging processes and make life predictions. Supporting this activity is the development of tools to diagnose and screen the state of a material to determine aging mechanisms. Studies are needed to explore the mechanisms of environmental stress cracking, one of the least-understood problems impacting polymer lifetime. This would include an investigation of the mechanisms of thermal and other types of environmental degradation in polymers. Characterizing long-term aging is also discussed as a priority activity in Chapter 3, Characterization of Materials.



3 Characterization of

Current Situation

Characterization of materials properties and performance is a critical part of materials development and processing. When developing new materials, researchers need to *characterize* the physical and chemical properties of the material. They must also be able to measure and test the functionality of the material they are designing (i.e., how will it perform in terms of strength, durability, and other qualities). During the processing or manufacturing of materials, effective monitoring and control is essential to obtain the quality and properties desired in the final product. This often requires measurement, or *characterization* of the material as it is being produced.

Great strides have been made in measurement technologies over the last two decades, and these have accelerated progress in many areas of the chemical industry, including materials science. Advances in areas such as superconducting magnets, multiple-wavelength lasers, multiplex array detectors, and atomic-force and scanning-tunneling microscopes have made substantial contributions to chemical analysis and measurement.

However, there are still many areas where capabilities are lacking, particularly for polymers and composite materials. In manufacturing of both chemicals and polymers compositional data is usually still obtained by technicians taking post-production samples. Real-time analytical measurements are not generally available. While there may be advanced, highly sophisticated instruments available for measurements, these have often been developed in isolation in R&D laboratories and cannot be readily applied in the manufacturing facility. Research-grade instruments often lack the robustness and general utility required for them to be used effectively by non-specialists in the chemical plant.

A large amount of information has been collected on the physical and chemical properties of polymers and composites. However, it is not consistently and readily available to researchers involved in developing new materials. Another limitation is that researchers involved in materials development lack good techniques for predicting materials properties based on structure data. In particular, materials characterization to the level of macromolecular architecture would help to resolve some of the issues of cross-linking, branching, and composition of polymers. There are also limitations in capabilities for characterizing multi-component materials, and determining physical properties from measurements.

Goals for 2020

The broad goals identified for materials characterization are shown in Figure 3-1. Many of these focus on overcoming the current limitations of systems for sensing and control of materials properties. Achieving on-line, continuous real-time monitoring is a critical goal for improving quality and performance in the manufacturing of new and existing materials. Closely connected to real-time monitoring is the ability to conduct such testing much more quickly than is possible with today's technology. Speed is particularly important in the plant where tests are conducted not by scientists highly familiar with the technology, but by skilled technicians attempting to optimize process parameters and daily operating conditions.

The ability to analyze very small variations in the structure and composition of polymers would greatly enhance control of polymerization processes. To achieve this entirely new technology may be needed, or significant modifications made to change the way existing characterization systems (e.g., spectroscopy) are used.

Understanding how materials age and perform over time is a critical goal for materials characterization, and it impacts the development of new materials as well as existing materials. A sound knowledge and prediction of the lifetime of materials would enable their use in many more applications where such issues are of vital importance (e.g., polymers as structural materials in buildings, bridges).

**Figure 3-1. Broad Goals for 2020:
Materials Characterization**

- Achieve on-line, continuous real-time monitoring
- Increase speed of testing by an order of magnitude
- Increase the speed of analyses by non-experts
- Analyze precisely very small variations in polymer structure and composition
- Miniaturize spectroscopic techniques
- Understand the long-term aging and liability of materials (accelerated aging)

Opportunities and Applications for Materials Characterization

Technology Opportunities

There are many opportunities for materials characterization to improve technology and expand markets (see Figure 3-2).

Improvements in materials characterization will allow better monitoring and control of the materials manufacturing process, and more accurate information on the performance and properties of the final product. The direct result will be improved first pass, first quality yield. Overall, better monitoring and control will help achieve six sigma performance, increase the safety of the manufacturing process, reduce waste (in-process and post-consumer), and subsequently increase yields and profits. There are particular opportunities for better control of colloid systems, multi-component mixtures, and interfacial properties.

Better materials characterization capability could impact the materials development process by enabling faster product development and cutting time-to-market. One example is the development of multiple techniques for the materials discovery process. New product development will be

Figure 3-2. Opportunities for Material Characterization	
Technology Opportunities	Market Opportunities
<p><i>Better Monitoring and Control</i></p> <ul style="list-style-type: none"> • Mass customization • Six sigma performance • Integrated total-system characterization • Early warning for on-line manufacture and in-service • Increased safety of manufacturing processes • Understanding/control of single and multi-component interfaces • Better control of colloid systems • Manufacture of complex assemblies (polymers and other materials) <p><i>Product Development</i></p> <ul style="list-style-type: none"> • Multiple methods for discovery of new materials • Faster product development 	<p><i>Life Sciences/Biotechnology</i></p> <ul style="list-style-type: none"> • Drug discovery • Medical diagnostics • Organ replacements • Living tissue interfaces • Truly biomimetic materials • Material production in living organisms <p><i>Consumer Products</i></p> <ul style="list-style-type: none"> • Electronics • Optical film • Biodegradable polymers • High (data) capacity storage • Polymer/material based sensors (packaging) <p><i>Infrastructure</i></p> <ul style="list-style-type: none"> • Fuel cells/batteries • Structural polymers

further enabled by the capability to manufacture complex assemblies containing polymers and other materials, being able to characterize mixtures of polymers, and innovative new areas such as material production in living organisms. Better characterization techniques will be especially important in life science applications (biomedical) where product liability is a critical issue. An example is material production in living organisms, which could open up significant biomedical opportunities.

Market Opportunities

Improvements in the ability to characterize materials could encourage expansion into many new markets in the life sciences, notably biotechnology, drug discovery and drug delivery systems, organ replacement, living tissue interfaces, and medical diagnostic tools.

Better understanding of polymeric materials and how they perform over time could lead to broader applications for polymers. Polymers could one day replace traditional construction materials such as wood, concrete, and steel in structural applications.

Barriers to Improved Materials Characterization

Technical Challenges

One of the most critical technical barriers in characterizing materials is the limitation of currently available instrumentation. The measurement of size and time in a sample remains one of the most difficult aspects. This problem is frequently compounded in materials that are multi-component and/or multi-phase, as these materials often cannot be analyzed by one scientist or specialty. Another important barrier is that there is no systematic materials approach to define infometrics (data mining). A consistent, effective method for the acquisition and organization of information and properties data would allow for faster process and product development.

Economic

There are several economic barriers that hinder improvements in the area of materials characterization. The highest priority barrier is that incentive for improvements is too diffuse. There is no single motivational factor for bringing about change. Since altering production procedures is both technically difficult and expensive, the motivation to do so without great economic benefit is very small. Many problems in the manufacturing arena can also be avoided instead of solved. This may initially seem like the most economically viable option, but many of the same problems return repeatedly, creating a decrease in profitability over time.

Translateability of Structural Properties

A critical barrier is the lack of capability for extrapolating physical properties from measurements. Overcoming this barrier could bring about major improvements in the characterization of materials and new materials development.

R&D Infrastructure

The largest hindrance in this area is the lack of communication between different researchers and disciplines involved in materials research. This lack of communication revolves around intellectual property rights as well as a general aversion to communication and change. In addition, there are always some difficulties in transferring technology from the R&D stage to commercial production, especially when altering production procedures is capital-intensive and costly.

Standardized Data

A significant barrier is the lack of a standardized data base for accessing information on existing and newly developed materials. A catalogue of available physical properties data and other information concerning materials would be an invaluable tool. Further compounding the problem is the lack of a set of standards for communication between scientists to facilitate “data swapping.”

Education

In academia, poor communication between researchers in the many diverse technical disciplines where materials research is conducted creates a barrier in the sharing of information and new discoveries. Collaborative interdisciplinary research is not widespread in academia or industry. Since materials research cuts across many industries (e.g., basic processing industries, biotechnology, and life sciences) the lack of interdisciplinary communication constitutes a significant limitation. Part of the problem is that materials scientists do not communicate well with professionals in areas that are very different, such as the life sciences.

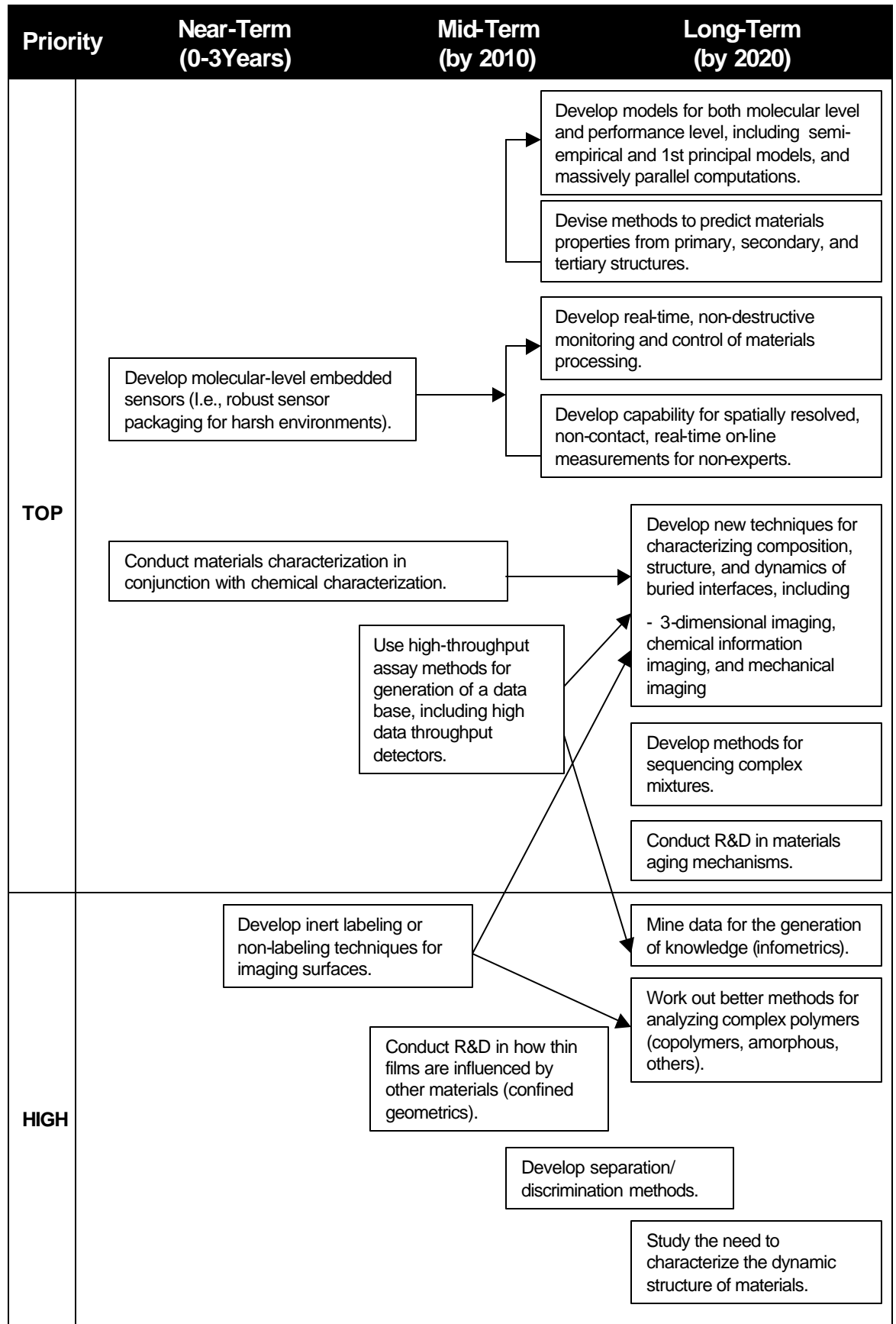
High Priority Research Areas

The priority research needed to foster improvements in materials characterization is shown in Figure 3-3. Research is organized by timeframe (when meaningful results and process improvements can be expected). A complete table of all R&D needs is provided in Appendix B.

R&D Tools

The research tools that can make the biggest impact in the area of materials characterization are new techniques for composition, structure, and dynamics for buried interfaces. Imaging techniques such as 3-D imaging, chemical information imaging, and mechanical imaging are a high priority. Another priority R&D tool is high-throughput assay methods for generation of

Figure 3-3. Priority R&D for Materials Characterization



databases. Closely connected is the need for data mining for the generation of knowledge (also known as infometrics). A key element in R&D tool development is that materials and chemicals characterization should be conducted in tandem, rather than in isolation, to provide a more complete picture of materials functionality and properties. Overall, development of new R&D tools will provide a source of input for a much-needed materials database, which has been identified as a critical limitation to materials characterization.

Real-Time Measurements

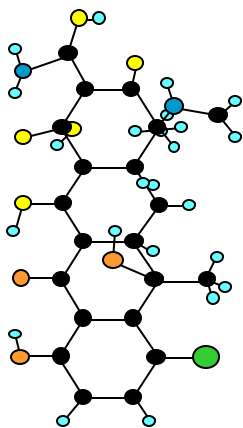
Measurement and control of systems operating continuously remain a challenge for the materials industry. Development of on-line, spatially resolved, and non-contact measurement techniques, especially those that can be used by non-experts, is an important need for materials processing as well as new materials development. One measurement technique is the development of an embedded sensor at the molecular level. Developing non-invasive control devices that are embedded in a material on the molecular level could completely change the nature of today's materials and how they are manufactured. Another important tool is the ability to make local physical property measurements on a nanometer scale. Note that most of the above needs are called out in *Vision 2020* as priority research areas.

Modeling and Simulation

Since modeling remains one of the most challenging aspects of technology, the research needs in this category fall into the long-term time frame. Modeling on the molecular as well as on the performance level will be critical to achieving industry goals. The development of semi-empirical models and first principal models will be an important breakthrough in this field. A need for massively parallel computation capabilities will increase as the accuracy of models increases. Models that are capable of predicting material properties from primary, secondary, and tertiary polymer structure are also needed. An area that has often been neglected (for polymers in particular) is material aging and lifetime analysis. Being able to predict and compare material lifetime is critical for application of polymers and other new materials in structural and transportation applications (aircraft, buildings, bridges). More detail is provided in Chapter 4, Materials Modeling and Prediction.

R&D Education

One of the greatest barriers to achieving goals was identified as the lack of communication between various disciplines. Exposure to collaborative interdisciplinary research on both the university level and professional level is needed to overcome this barrier. Requirements for obtaining a Ph.D. in chemistry or engineering should be diversified and broadened. Students in the physical sciences should be exposed to the language and approaches of the life sciences. This will ensure that new graduates are well-read and prepared to handle the challenges of the materials industry.



4 Materials Modeling

Current Situation

Computational Techniques

Computational techniques have improved dramatically over the last two decades along with the revolutionary advances in computing power. It is now possible to use computational methods to address a number of practical engineering and design issues in chemical processing. Computational techniques are being used to complement, guide and sometimes replace experimental measurement, reducing the amount of time and money spent on research to bring ideas from the lab to practical application. The growing interest of larger firms in computational techniques has resulted in the growth of software vendors that specialize in user-friendly modeling packages for chemical, biochemical and biological applications.

In the pharmaceutical industry computational methods have played an important role in structure-based drug design, most recently in the development of the current generation of HIV protease inhibitors. In the chemical industry considerable effort has been expended on using computational techniques for the design of homogeneous and heterogeneous catalysts. While useful, the application of computational techniques to heterogeneous catalysts has met with somewhat limited success because of the types of atoms involved (transition metals) and the lack of techniques for dealing with them. Computational tools have also been used with varying success for applications involving adhesives, coatings, polymers, and surfactants. However, many of these tools are limited when applied to the design of polymers.

Computing Power

The availability of computer hardware capable of handling highly complex computations has increased rapidly over the last five years to support the development and use of advanced computational software. Development of vector and vector/parallel machines, RISC architectures and powerful desktop computing, and more recently, massively parallel computing systems based on lower cost RISC processors is allowing the solution of problems that were previously impossible to solve. Moderate cost, high performance workstations have made it easier to generate input data and to analyze and view the results of large calculations as well as perform reasonably complex calculations at the desktop.

At present, the highest available computing performance is found on massively parallel processing (MPP) computers with approximately 100 gigaflops of sustainable performance using a highly tuned (relatively flawless) code, with 50 gigabytes of memory and 1 terabyte of disk storage. The current cost for a system with these capabilities is approximately \$20-25 million. A typical system with this performance has distributed memory with about 500 processors. With these systems the

greatest technical issue is dealing with non-uniform memory access (NUMA) and the associated latency for data transfer between memory on distributed processors. Present single processor workstations have on the order of 250 megaflops of peak performance, with 512 megabytes of random access memory and 10 gigabytes of disk memory. The cost of single processor workstations is approximately \$100,000.

Goals for 2020

By 2020, one objective is to have modeling completely integrated into the R&D process, with all companies routinely using models to guide product and process design (see Figure 4-1). The successful use of models for this purpose will enable substantial reductions in the development cycle (from concept to market), and greatly reduce the need for costly and time-consuming experimentation. Experiments will be better targeted towards product development, and will be more successful because experimentation is guided by modeling. Experiments will be used to validate and improve models, rather than as a source of data. By 2020, models will enable researchers to more easily explore beyond current theory and experiment and will be the basis for the discovery process more than 75 percent of the time.

Process engineering will be greatly improved by achieving goals for modeling. Models will be fully integrated with processes, enabling the prediction and analysis of the properties of at least 50 percent of process streams. By 2020, the goal is to have models available for ideal gas processes and single liquid and solid phase systems.

**Figure 4-1. Vision and Goals for 2020:
Materials Modeling and Prediction**

- All U.S. companies use modeling from the beginning of the R&D process.
 - Large companies each have 30 modelers by 2010.
 - Small companies each have 2 modelers by 2020.
- Reduce the development cycle by 50% by 2020.
- Modeling and experimental labs for data will be unnecessary.
- Experiments will be focused on model validation and improvement.
- Theory, computation, and experimentation will be fully integrated.
- Half of all scientists/engineers will be educated in computational materials science.
- Modeling will be to materials development as architecture/civil engineering is to building buildings.
- By 2005, modeling and prediction will be integrated with business knowledge.
- Models will be used to explore the limits of what is fundamentally possible beyond experiment and theory. In 2010, this will be done 50% of the time; in 2020 it will be done 75% of the time.
- It will be possible to predict properties by knowing formulation and processing conditions for 50% of all major process streams.
- Models will be fully integrated, yielding detailed process engineering models (CFD).
 - For ideal gas-like processes, this will occur by 2010.
 - For single phase liquid or solid systems, this will occur by 2020.
- New ideas will be explored with models versus experiment or theory 10% of the time in 2010 and 20% of the time in 2020.

Opportunities for Modeling and Prediction

Improved models and predictive capabilities for materials offer significant opportunities to improve materials design and functionality (see Figure 4-2). Prediction of morphology is a principle area of interest, particularly for multi-component, multi-phase materials. Another important opportunity is first principles prediction of a wide range of soft materials. There are many cases where first principles predictive capability could help broaden potential applications of these materials.

There are many areas where modeling capability is currently limited, but which could benefit greatly from computational tools. These include health, safety and toxicity issues related to new materials, lifetime (aging) of materials and equipment, life cycle analysis of materials, and reliability and failure mechanisms. Advances in all these areas could lead to the development of new materials that are better designed for specific applications, products with increased reliability and service life, and less environmental impact.

Figure 4-2. Opportunities for Materials Modeling and Prediction

- Prediction of morphology of multi-component, multi-phase material as a function of formulation and process conditions
- Prediction of mechanical and rheological properties as a function of morphology for many types of materials
- First principles prediction of soft materials
 - blends
 - foams
 - block co-polymers
 - graft co-polymers
 - semi-crystalline polymers
 - liquid crystalline systems
 - emulsions
 - dispersions
 - colloids
 - polymer melts
 - filled polymers
 - composites and nanocomposites
 - amorphous material
- Combinatorial materials science
- Mesoscale modeling
- Lubrication and tribology
- Nanotechnology
- Addressing health, safety, and toxicity issues related to materials
- Prediction of ultimate fate and service lifetime of equipment and entire plants
- Prediction of ultimate fate and transport of materials
- Intelligent materials
- Prediction of properties from structures
- Software
- Reliability and failure
- Chemical kinetics and catalysis
- Materials synthesis
- Interfacial phenomena
- Biomaterials

Barriers to Improved Modeling and Prediction

Fundamental Knowledge

The fundamental knowledge required to create more effective materials models is critically lacking in some areas. The most important of these are bridging techniques, interfacial phenomena, force fields, dilute solutions, and long-term chemical and physical aging. Another important issue is the lack of practical experience in successfully creating new mesoscopic/ mesoscale models.

Particular problems are encountered in modeling multi-phase fluids, where models have correlative and phenomenological capability but not necessarily predictive power.

Hardware/Software

For many current modeling applications, computer hardware is either not fast enough, or is too expensive for the speed required. Another important limitation is that more attention is being focused on making advances in hardware rather than improving the basic algorithms needed to increase overall modeling capability. A contributing factor is the lack of standardization of software architecture, which makes it difficult to transfer codes between companies and/or researchers in the field.

Implementation

Once models have been developed, a number of issues may arise that preclude their more widespread use. The most critical of these is experimental validation. Validation is often inadequate, which leads to uncertainty and unreliability in predictions. There is a significant lack of experimental data available for model validation, partly because of the time and expense involved in collecting this data. Methodologies in molecular modeling are not adequately validated, and most methods across a range of models are not sufficiently accurate. Another issue in using available models is that integration of the models to plant-wide operational objectives is very limited. More effort is needed to create models that are focused on solving the practical problems that arise in the plant environment.

Structural

It is often difficult to integrate the results of modeling activities into an organization, which limits their effective use. In many smaller companies, modeling is not considered because of the high associated start-up costs. All too often the corporate philosophy is that experiments are better and cheaper than creating models. This is partly because corporate decision-makers often have an experimental background, rather than theoretical. In general there is a lack of funding for modeling programs, and often a lack of experienced modelers. Some of the best and most knowledgeable in the field leave modeling for higher paying careers.

Model development often lacks the multi-disciplinary team approach (mathematics, engineering, chemistry, physics, computer science) required to optimize success. Another issue is that modelers doing different levels of modeling (mesoscale, atomistic scale, and so on) speak different languages and don't communicate effectively.

Education

A critical issue is that many scientists and engineers are not very familiar with models, and lack the mathematical and scientific method background to understand and use models. Part of the problem is that modeling is taught as a separate entity from most disciplines, and many do not enter the field because theory is not "exciting" and higher-paying careers are available.

High Priority Research Areas

The priority research needed to foster improvements in materials modeling and prediction is shown in Figures 4-3 and 4-4. Research is organized by timeframe (when meaningful results and process improvements can be expected). A complete table of all R&D needs is provided in Appendix B.

Methods Development

In the near-term, top priorities are the development of accurate potentials, better methods for mesoscale modeling, and hybrid and quantum techniques. Supporting research is needed in parallel algorithms and implementation, as well as new mathematical techniques for molecular modeling (e.g., multi-grid, multi-scale). Another top priority is a multi-faceted, multi-disciplinary effort coordinating theory, modeling and experimental research on interfacial science. Top priority topics in this on-going activity are aqueous systems, polymer liquid crystalline interfaces, polymer interface with inorganic solids, multi-phase multi-component systems, dissimilar surfaces, biomaterials, filled polymers, and nanocomposites.

Theory

Improved bridging techniques have been identified as the highest priority research area in theory development, and one that should be on-going over the next 10 to 15 years. Of particular importance are bridging length and time scales, mapping and reverse mapping, and renormalization as a bridging link. A top priority, near-term activity is the development of basic theory for materials science. Improved theories are needed to support modeling of materials at all levels. Other priority topics are better theories and modeling methodologies for non-equilibrium conditions, and determining how processing affects the ultimate properties of materials. Processing creates the material's microstructure, which ultimately determines final properties.

Specialty Materials

A high priority research area that should be on-going over the long-term is developing modeling and predictive capability for crystal formation in semi-crystalline polymers. Research is also needed to model materials that are very important to the industry but are currently poorly defined (e.g., carbon black, asphalt).

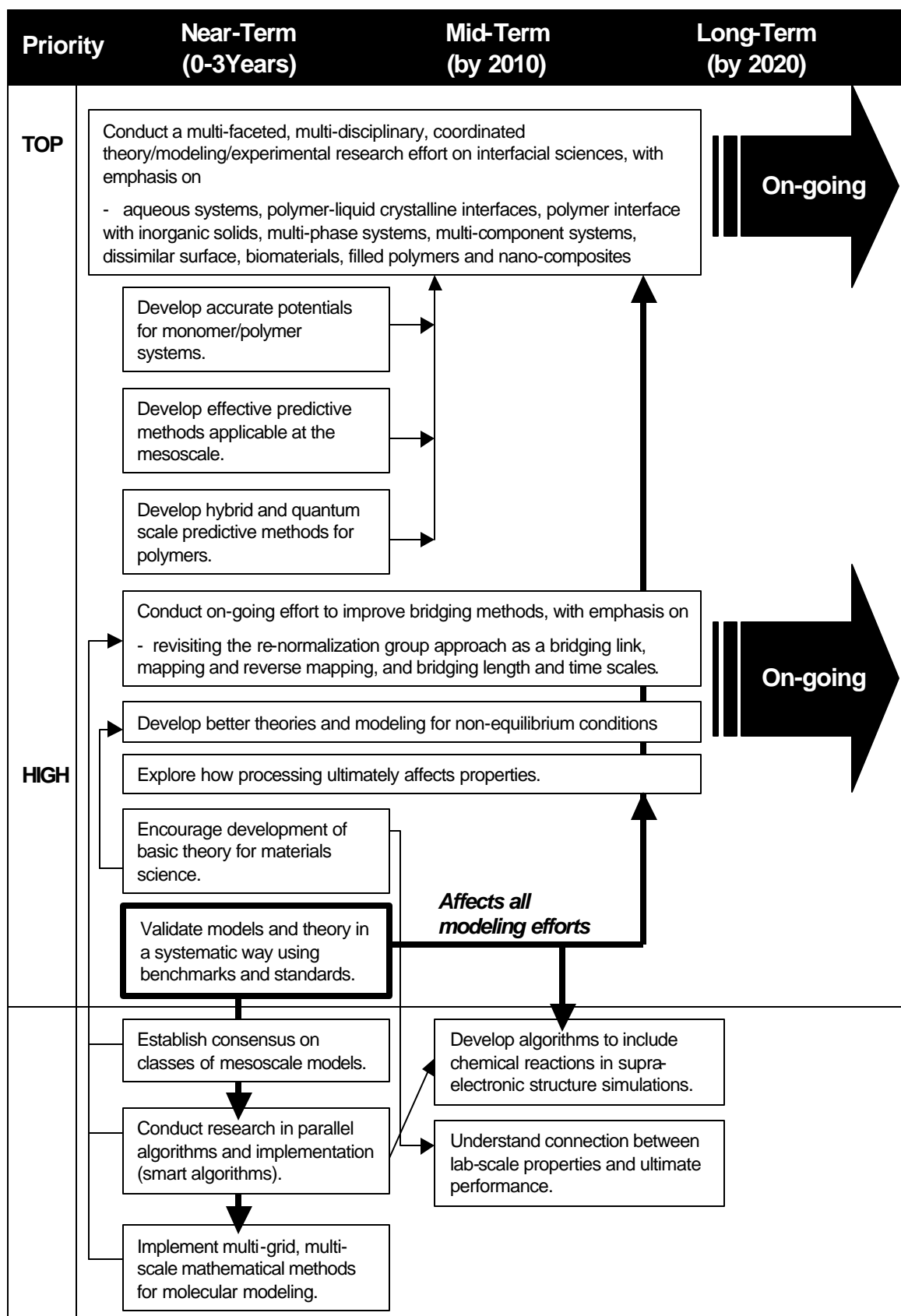
Enabling Tools

There are a number of enabling tools that should be further refined to support model development. The most important of these are improved data mining and discovery tools that enable the user to interact with data in a useful way. A central, publicly-accessible repository of data and validation tools is also a high priority. Standards for data structure, data input/output, and interfaces should be developed in tandem with a data repository.

Validation

A top priority is to conduct model validation in a systematic way using benchmarks and standards. Validation is critical to improving the reliability of model results and achieving more widespread acceptance and use. One approach is to implement model "best practices" through a research partnership (an example is the European Framework Five) to provide public validation of deliverables.

**Figure 4-3. Priority R&D for Modeling and Predictions:
Methods, Theory and Validation**



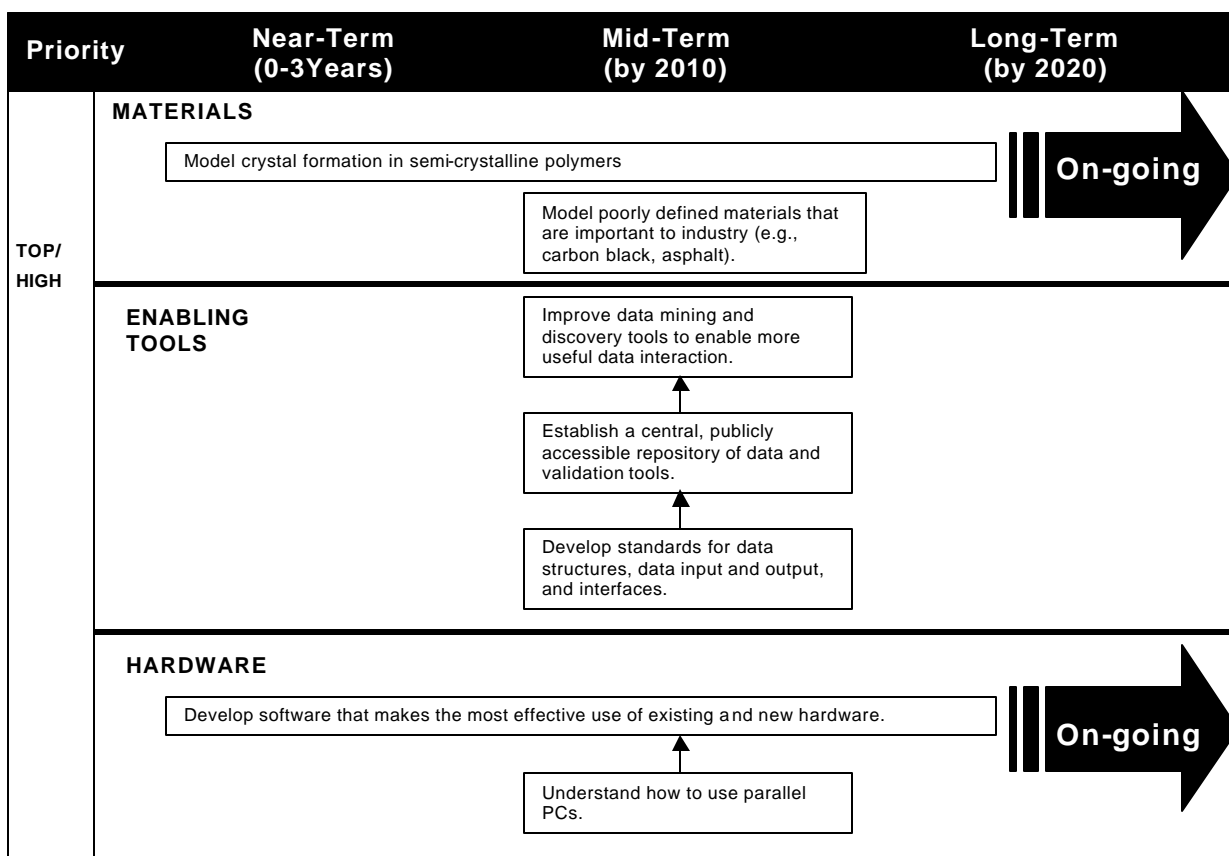
Hardware/Software

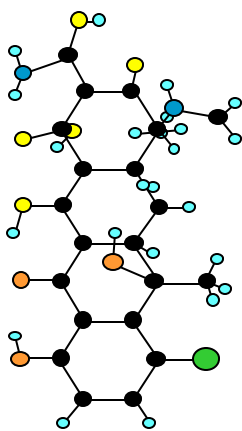
Hardware development is proceeding at a rapid pace outside the chemical community. However, better understanding of how to use parallel PCs in materials modeling applications is needed. Software is also needed to optimize the use of existing and new hardware.

Education

Some modifications are needed in academia to increase the pool of talented scientists and engineers interested in modeling. A high priority for the near-term would be to better integrate modeling and simulation techniques into undergraduate and graduate curricula. Another approach, which addresses the problem of inter-disciplinary knowledge, is to include an engineering course as part of the chemistry PhD program, and ensure that Master and PhD academic research projects include modeling activities.

**Figure 4-4. Priority R&D for Modeling and Prediction:
Materials, Hardware and Enabling Tools**





5 Additives

Current Situation

The processing of polymers and their performance can be greatly enhanced through the use of additives. Additives also provide the manufacturer with an opportunity to tailor polymers to a specific application. There are many classes of additives used to control physical and chemical properties, as shown below. Additives currently exist to meet some of the properties illustrated, but there are still many new opportunities to be explored and improvements to be made.

Desired Properties and Performance of Additives

- | | |
|---|---|
| • Antiblock/slip agents | • Flame retardants |
| • Antioxidants, thermal and UV stabilizers | • Heat/distortion stabilizers |
| • Antistatic and other electric response | • Impact modifiers |
| • Biocides (biostabilizers, biostimulants, and biocompatibility) | • Light stabilizers |
| • Chemical blowing agents | • Lubricants/mold release agents |
| • Coupling agents | • Slip additives |
| • Tackifiers | • Friction reduction |
| • Peroxides and cross-linking agents | • Nucleating agents |
| • Clarifiers | • Plasticizers |
| • Spectral control (vision enhancement) | • Fillers and reinforcement agents |
| • Catalyst stabilizers-deactivation (catalytic, co-catalytic, metals) | • Compatibilizers |
| • Processing aids (anti-lubricant) | • Colorants and pigments (inorganic and organic optical response) |
| • Surface modification | • Hydrolysis stabilizers and inhibitors |
| • Barrier properties | • Anti-fog |
| | • Anti-dirt |

Processing additives are used to reduce internal friction in the molten polymer (lubricants), change polymer morphology and increase thermal conductivity (nucleating agents), remove excessive heat (endothermic blowing agents), and to prevent thermal decomposition (antioxidants). Some additives enhance the appearance (optical brighteners) or performance of the final products (flame retardants, antistatic agents, light stabilizers). Modifying polymer properties and appearance with additives is typically more economical than the introduction of a new polymer component.

Polymer additives are one of the fastest growing segments of specialty chemicals, with forecasted growth of 5.5 percent per year, roughly 1.5 times global economic growth, to a total of 8 billion

pounds by 2001.³ The additives market has undergone significant change (thirty-five major acquisitions over the last five years) and achieved global sales of nearly \$15.2 billion in 1996. These dramatic changes are being driven by: the strong drive for shareholder value, globalization, higher performance requirements, and meeting regulatory and environmental demands. Nearly all major polymer additive multinational firms are based in Europe or North America, and the largest consumers are in the Asia/Pacific region. Many large firms are planning aggressive Asia/Pacific expansion plans, which could force large numbers of small suppliers, especially in China, to expand, partner, and/or consolidate to remain competitive. To remain competitive, technology development will be a strong component in the future health of the domestic industry.

Technological innovation in additives focuses on both performance and environmental needs. For example, light stabilizers and antioxidants are under development to improve the short- and long-term performance of polyolefins. Reduced metal and metal free heat stabilizers for PVC resin illustrate how new technology is being developed to address environmental concerns. In other areas, the issue of halogenated flame retardants (potential ozone depleters) is catalyzing the search for non-halogenated alternatives such as phosphorus compounds, melamines and inorganic materials.

Goals for 2020

Goals for additives focus on improving the performance and cost-effectiveness of polymers, and subsequently achieving greater application and use of these materials (see Figure 5-1). Goals for performance include improving material life time in service so that it is competitive with other materials. Additives can also be used to increase the cost-effectiveness of producing and using polymers by lowering total integrated costs. Important goals are to use additives to create entirely new properties that are not currently available, as well as enhance existing properties. Examples are noise-suppression capability, blendability, and lighter weight. Additives can help create new polymers that are easier to model, and are environmentally friendly (e.g., recyclable, bio-degradable).

Figure 5-1. Vision and Goals For 2020: Additives

- Design and create additives with critical functionality to meet needs in 2020
- Expand usefulness of polymers through the use of additives
- Increase cost-effectiveness through additives (e.g., total integrated cost)
- Ensure that polymer lifetime (e.g., control, assurance and predictability) is as good as other materials in terms of cost and performance
- Use additives to create materials with enhanced properties and functionality, such as
 - Noise-suppressing, blendable, more colorful, cheaper, smaller, lighter, more convenient to use, longer life, environmentally friendly

³

“Dramatic Changes in the Plastics Additives Market,” January 19, 1998. Townsend Tarnell, Inc.

Opportunities for Additives

Market Opportunities

Additives could be used to promote the use of polymers in a number of areas (see Figure 5-2). One of the roles additives can play in materials development is to improve the properties of polymers so that they meet the performance requirements needed for brand new applications. These range from innovative applications like photochromic greenhouse windows to polymer houses and bridges. Structural polymers are an important application area where there is huge room for growth, if polymers can be developed to meet structural specifications and aging requirements. Polymers that are truly ‘weatherable’ would open up many opportunities in structural as well as consumer applications. Important examples are low delta e dark-colored polymers that have mechanical stability, and recyclable polymer components that could serve as alternatives to poly vinyl chloride (PVC).

Technology Opportunities

Improved additives can help to enable a number of important advances in new materials technology (see Figure 5-3). Among these are adjusting of properties to attain greater recyclability; controlled biodegradation; additives to indicate physical phenomena is occurring, such as oxidation; and polymers that can tolerate high temperature melt fabrication and processing.

With new additives it could be possible to make transparent polymers that are much less permeable, which could have important implications for polymers as a packaging material and possible replacement for glass. Biologically-active additives could open up new markets for disease control and biological protection materials. Smart additives could be used to create innovative control technology.

Exhibit 5-2. Market Opportunities for Additives

- Truly “weatherable” (i.e., low delta e) dark-colored polymers via additive technology (i.e., with color and mechanical stability so the polymers does not fall apart
- Photochromic greenhouse windows
- Clear polymers sheet with a 20-year life
- Structural polymer systems (e.g., composition) that are stable and not subject to property deterioration (chemical change) over a 30 year life-time (e.g., polymers houses, bridges)
- Rigid foam
- Blends and alloys
- Tough, “weatherable” recyclable polymers components (i.e., instead of PVC)
- Commodity polymers with the properties of an engineering thermopolymers. (e.g., obtaining the modulus-toughness of acrylonitrile-butadiene-styrene with polypropylene)
- New anti-static additives for “future polymers”
- Additives for all-polymer solar energy converters
- Additives that allow/stabilize recycle/reuse of multi-polymer blends
- Improved medical devices

Figure 5-3. Technology Opportunities for Additives

- Additives to indicate physical phenomena (i.e., oxidative, chemical, electrical)
- Nanoparticle fillers—(provides more interface to increase effectiveness)
- Anti-static control without optical, coloring, or environmental effects
- Property enhancers at low addition levels
- Adjustable properties through additive concentration to enable recyclability
- Transparent polymers with a 10-fold reduction in permeability via additives (e.g., H₂O, O₂, CO₂, etc.)
- Additives that shift or respond to “light” and/or “energy” besides ultraviolet
- Biologically active additives for disease control and biological protection
- Completely biodegradable polymer system without any environmentally unfavorable consequences (i.e., low toxicity)
- High temperature stabilizers for 300°C to 400°C melt processing/fabrication
- Additives that enable controlled biodegradation of polymers
- The capability to engineer thermopolymers with a “continuous use temperature” >200°C
- Quality control (smart additives)

Barriers to Improved Additives

Interfacial Interactions

Interfacial science for polymer interactions is significantly limited. Understanding how polymers react with their external environment, as well as with additives, fillers and composite elements, is critical to predicting how the material will perform as a product and during processing. Areas where knowledge is seriously lacking include surface chemistry, filler structure and relationship to material properties, the dynamics of polymer processing (especially how fillers and additives react), and the fundamentals of physics and chemistry in interfacial regions. Other important limiting factors include the inability to toughen and reinforce polymers simultaneously, and the lack of understanding of how impact modifiers work.

Modeling, Characterization and Prediction

The most critical barrier to better modeling and characterization of polymers is the inability of existing molecular models to predict additive-polymer system behavior. Contributing to this basic limitation is the general lack of understanding of the tools of multi-scale modeling. Currently available analytical tools overall are inadequate for polymer modeling, and fundamental understanding to create better tools is lacking.

Current Additives

A major limitation of current additives is that thermal stabilizers effective at temperatures greater than 250°C are not available. There are also a limited number of non-halogen gas phase flame retardants and stable, light-fast, non-toxic pigments and dyes. It is also difficult to optimize the use of fillers as the design and control of filler morphology is limited.

Financial Commitment

In general, the tendency of corporate decision-makers toward the short-term business view is a deterrent to financial commitment to higher-risk research in additives. A contributing factor is the management view of growth by acquisition rather than by research, which is manifested by an overall lack of business management support for research. Other factors include the large capital investment that may be required for new technology, and the high cost of testing the toxicity of new additives.

Industry-Academic Interface

The limited understanding and connection of academia to the practical problems experienced in industry limits successful research collaboration. Further exacerbating the problem is there is little understanding of the true value of industry-academic partnerships in pre-competitive research areas. Other factors include the fact that fewer people in industry want to learn in detail about technology, and that fewer graduates are entering the sciences than business fields.

Intellectual Property Issues

Research to develop better additives is often inhibited by the corporate philosophy that the competitive position must be protected, and that collaboration may lead to compromised intellectual property rights. It is perceived that establishing ownership of intellectual property may be difficult in such situations. The result is that technical advances may be slow to come to fruition. Another issue is the lack of a fast-track route to commercialization of new additive chemistry, especially when compared with patent life. Concern over intellectual property also makes it difficult for some companies to form CRADAs (Cooperative Research and Development Agreements) with government laboratories as well as other partnerships.

Regulatory/Government

The current regulatory environment can add substantially to the cost of development of new additives, and the situation is worsened for smaller companies with less to invest. There is also a perception that the government funds projects that benefit only the partnering companies, and these may be anti-competitive when exclusive rights are given to the company conducting the research.

Information Management

A major barrier to additives development is the wide dispersion of the knowledge base. Many organizations have knowledge, but availability is limited due to the proprietary nature of the data. It is also difficult for researchers to keep abreast of and assimilate the large volume of newly published data.

Communication

The inability of suppliers to articulate and understand risk management associated with new additives as well as new chemistry and science limits both use and development of additives. Additive manufacturers also don't communicate very well the concept of cost versus cost-effectiveness in selling users on new additives.

High Priority Research Areas

The priority research needed to foster improvements in materials modeling and prediction is shown in Figures 5-4 and 5-5. Research is organized by timeframe (i.e., when meaningful results and process improvements can be expected). A complete table of all R&D needs is provided in Appendix B.

Structure-Property Relationships

Predictive modeling of structure-property relationships for additives and polymers is a top priority. A seamless multi-scale portfolio of computational methods that will allow the study and prediction of polymer properties is a critical need and will require a long-term effort. Modeling systems that can handle multi-phase systems on a scale large enough to predict physical properties are also a top priority. In the mid-long term, research is needed to understand the interfacial interactions and surface chemistry of additives. Knowledge of fracture mechanics, and

**Figure 5-4. Priority R&D for Additives:
Structure-Property Relationships, Characterization and Processing**

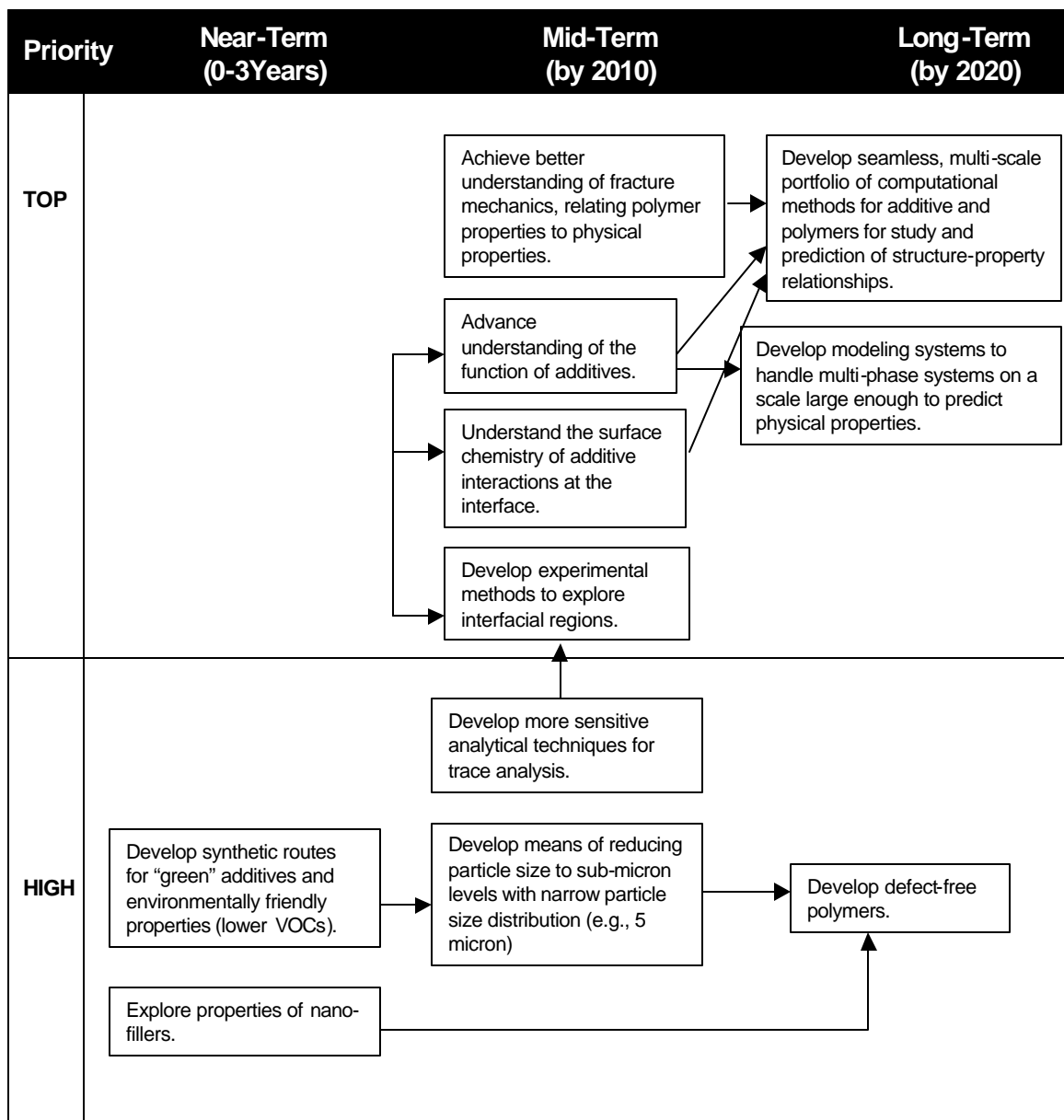
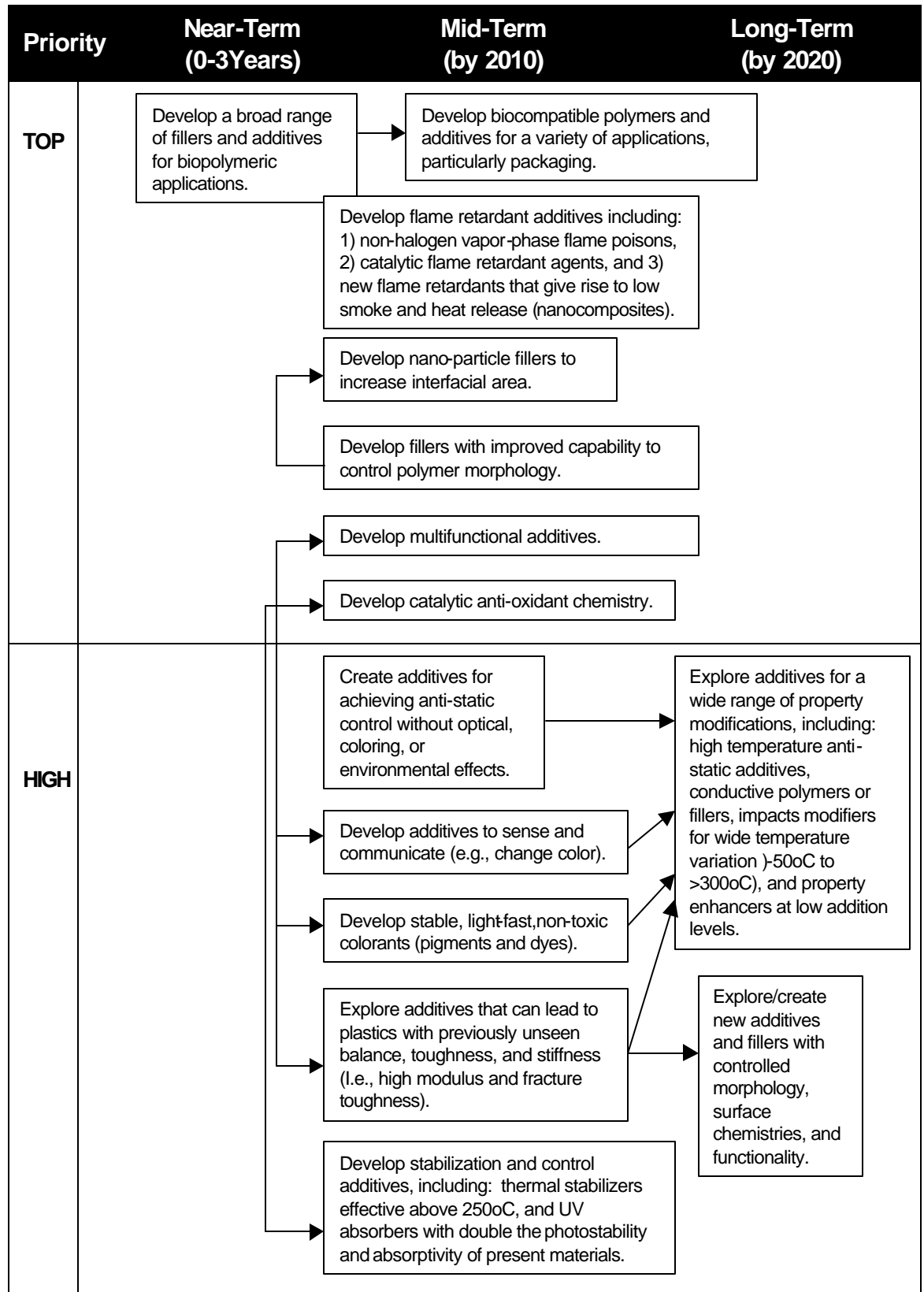


Figure 5-5. Priority R&D for Additives: New Additives



how to relate polymer properties to physical properties is also a top priority. In general, research to advance understanding of the function of additives is a priority and will foster improved additive design and performance.

Characterization Methods

To support modeling and prediction activities and additive development, experimental methods to explore interfacial regions are a priority research need. To assess material performance, better and more reliable accelerated aging techniques are needed, along with more sensitive analytical techniques for trace analysis.

Advanced Processes

A high priority research area is the development of processes that produce defect-free polymers. Advanced processes can also be made possible through the development of methods to reduce particle size to submicron levels with a narrow particle size distribution (e.g., 0.5 microns). A more general research priority is the exploration of new synthesis routes for “green” or more environmentally-friendly additives, particularly those that lower emissions of volatile organic compounds (VOCs).

New Additives

Property modification is a priority research area for the development of new additives.

Research is needed to explore nano-particle fillers, which can increase additive effectiveness through greater interfacial area. Fillers with improved capability for controlling the morphology of polymers is also a key area for study. Additives are needed to create polymers with previously unseen balance, toughness, and stiffness (e.g., high modulus and fracture toughness). Other important property requirements include stable, light-fast, non-toxic colorants (pigments and dyes), and impact modifiers that can withstand processing at extreme temperatures ($>300^{\circ}\text{C}$ and -50°C). A topic of special interest is the development of property enhancers or fillers that work at low addition levels.

Additives that impart **flame retardant** properties are an important area for research. Non-halogen vapor phase flame poisons, and catalytic flame retardant agents are top priorities. Other areas of interest are flame retardants that give rise to low smoke and heat release (e.g., nanocomposites), and self-extinguishing thermopolymers.

Additives are needed to increase **stabilization and control** of polymers. A top priority is the exploration of anti-oxidant chemistry that can be catalytic. Another important approach is the development of thermal stabilizers that are effective at higher temperatures ($>250^{\circ}\text{C}$). Ultraviolet (UV) absorbers may provide another means for stabilization and control. Research is needed to develop UV absorbers with at least double the photostability of present materials and double the absorptivity of current absorbers.

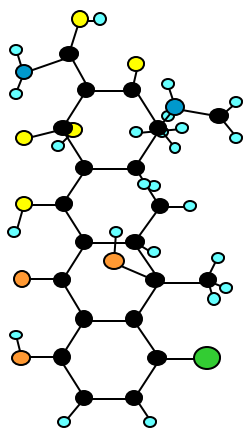
An important and emerging area for research is **bio-compatibility**. Development of bio-compatible polymers and additives could open up new markets in biomedicine and bioprocessing, and is a high priority. Biobased and recyclable polymers for a variety of packaging operations can also be made possible through the development of new additives. New bio-compatible additives can lead to completely biodegradable polymers that have no environmental consequences.

Multi-purpose additives can be developed to reduce material costs and impart improved properties. A top priority is the development of multi-functional additives (e.g., electrical conductivity, crystalline, properties other than color). Other priorities include additives to sense and

communicate (e.g., change color), that can indicate physical phenomena (oxidation, chemical and physical changes), and functional stabilizers that work via a speciality co-monomer.

Cooperation Between Industry, Academia and Government

A concerted effort is needed to develop more realistic global environmental regulations. Regulations are often quite different in competing nations, which creates an imbalance in production costs and fair market price. To foster more effective R&D collaboration, better industry-university partnerships in research and teaching should be explored. Better incentives should be developed to encourage industry to enter into joint partnerships with academia.



6 Disassembly, Recovery, And Recycling

Current Situation

Recovering and reusing (recycling) the original materials used to manufacture industrial and consumer products is an environmentally sound idea that has been practiced for many years. Polymer recycling, which first gained widespread acceptance in the late 1980s, has grown steadily and is flourishing. More than 1,400 quality products made with or packaged in post-consumer recycling polymers are now commercially available, including disposable cameras, battery casings, films and bags, crates, x-ray film, park benches, sweaters, video cassettes, detergent and soft drink bottles, and toys. The number of polymers recycling businesses has tripled since 1990, with more than 1,850 businesses handling and/or reclaiming post-consumer polymers. During the same period polymer bottle recycling increased six-fold, with about 1.5 billion pounds recycled in 1998. More than 1 billion pounds of non-bottle consumer polymers were also recycled that same year.⁴

New technology for polymer recycling is emerging continuously. Carpet manufacturers are introducing technology that will enable the recovery of carpet fibers and underlayments. Computer and business equipment manufacturers are testing the recovery of polymeric housings and components. Polymers lumber made from recycled polymer containers is gaining in popularity as a durable, efficient alternative to wood in decking and garden applications.

Disassembly can be an integral component of recycling. Disassembly most often refers to products that are designed to be disassembled after use and recycled to produce a comparable product. Since industrial ecology⁵ became popularized in the 1980s, the concept of “design for disassembly” or “design for recycle” has received increasing interest. The concept is that durable goods such as automobiles, television sets, computers, refrigerators, and washing machines, could be returned to the manufacturer when they are no longer usable, and be disassembled and recycled. The disassembled parts would then be used to create comparable products (e.g., another washing machine), not products of lesser value (like road paving or benches). Few products are currently designed to be disassembled, although research and interest in this area continues. The American Plastics Council, for example, is currently working with several private firms to develop and demonstrate new technologies that will allow the identification of polymers in durable goods (e.g., automobiles, computers, major appliances) and subsequently allow for their

⁴ American Plastics Council. *1998 Recycling Rate Study*.

⁵ Study of how humans can use natural resources, but in such a way as to protect human health, the health of natural ecosystems, and the health of future generations of plants, animals and humans.

recovery and recycling. A number of life cycle studies have also been done to determine the economic viability and benefits of design for disassembly.

The technology and infrastructure for polymer reclamation and processing is currently much greater than the supply of post-consumer polymers. Manufacturers need a steady supply of recycled polymers from consumers to ensure they can meet demand for their products. Consumers are not recycling to the fullest extent possible, and better, more cost-effective sorting technologies are needed.

Goals for 2020

The broad goals for disassembly, recovery, and recycling technology are shown in Figure 6-1. The goals for the industry are related to increasing economies of scale for polymers recovery and reuse through technology and management; industry and public responses to foster the market; and expansion of the material source base as well as uses for recycled polymers.

Figure 6-1. Broad Goals 2020: Disassembly, Recovery, and Recycling

Industry-wide Goals

- U.S. chemical industry is a global leader in recycling
- All materials and products are designed for recovery
- Of all the polyethylene (PE) produced, 20 to 30% is recycled
- Landfill need for polymers is reduced by 50%
- Automobiles are 100% disassembled and recycled
- The majority of polymers are produced from renewable resources
- Recycling promotes environmental quality and provides an expanding number of jobs

Technology Development Goals

- Polymer reuse in original applications is maximized
- Recovered polymers are a valued raw material for new polymers (too valuable to burn)
- Industry efficiently categorizes and separates material into useful and pure components
- A recycled polymers specification center establishes consensus on performance standards for recycled polymer use market-wide and on polymer rationalization

Market Development Goals

- Innovative legislation (not mandates) promotes recovery and creates market predictability for post-use material managers and recyclers (e.g., disposal fees and product specifications)
- The recycled polymers market is economically competitive with the non-recycled/conventional material
- Recycling companies are widely dispersed and profitable
- Polymers are viewed as the material of choice by the public and environmentalists
- Chemical engineering education curriculum includes recovery and reuse
- U.S. chemical industry uses generally accepted accounting principles for internalizing social and environmental costs

Energy Source Goals

- Polymers used as a fuel are combusted efficiently and with low emissions
- Polymers are gasified with low emissions
- Old polymers are recovered from every major market sector

Opportunities and Applications for Disassembly, Recovery and Recycling

Recovered materials and techniques for recycling have the ability to affect both current and future practices in the post-use material industry and in manufacturing. Figure 6-2 lists a number of opportunities where better and more efficient processes could expand the use of waste polymers and create new markets. Important post-consumer waste streams that have not been tapped include carpets, construction materials, diapers, rubber, and demolition materials.

Figure 6-2. Opportunities for Disassembly, Recovery, Recycling and Renewables

- As a source of polymeric feedstock, recover construction and demolition material (e.g., PVC and wood), carpet, tires, rubber, diapers, and other products in landfills
- Focus on commercial sector for more predictable waste streams (e.g., recycle cutting waste from polyester and cotton plants)
- Select biologically derived polymers and monomers for biodegradability (e.g., for cellulosic-derived diapers)
- Develop methods to decolorize recycled polymers
- Separate post-use material entering landfills for ease of future recovery (e.g., landfills charge less for separated material)
- Capture the value of post-use materials through public-private partnerships
- Convert mixed polymer, food, diapers, and paper to intermediate source of energy in small-scale distributed processes

Barriers to Expanded Use of Disassembly and Recycling

Design for Recycle

Products are almost always designed without consideration of what happens at the end of their “useful” life. In many cases, recycling is inefficient because of the polymer mix and processing requirements for materials that have not been designed to be recovered and reused. Designing products for post-use material recycling facilitates disassembly and recovery and increase the value of the recycled material.

Collection

Collecting post-use material is a significant challenge for the industry. The critical barriers to an expanded, viable market for polymer recovery include the cost of collection, and the availability of used material in large enough quantities to have a desirable and recoverable polymer mix. Further, recovered materials must be consistently available (quantity and quality) so the industrial processors have a dependable supply of feedstock.

Identification and Sorting

During or after the time post-use material is collected, the polymer is identified and sorted accordingly. Once sorted, the polymer must be disassembled and separated into polymers or useful agglomerates. The inability to identify polymers quickly and accurately slows the process and leads to supply streams having both desirable and undesirable polymers. The resulting range of polymer types in post-use material constitutes a significant recycling barrier. For example, film packaging of mixed composition uses ten or more polymers, which is too many to recover. Overall, the highest priority barrier is the lack of processing capability to separate polymers with high enough yields and purity to produce the feedstock industry needs.

Product Purity and Process Flexibility

Product purity is limited by the inability to remove or prevent contaminants, variability of the post-use material supply stream, and the technology and processing flexibility needed to respond to supply variability. The primary barrier in this category is the inability to use chemistry to affect the physical properties of the supply stream. Existing process chemistry is insufficient to contribute to physical separation of the incoming stream.

Cost of Process and Scale-up

Processing post-use material for polymer and monomer recovery is expensive, and obtaining economies-of-scale through scale-up of the operation presents challenges to the industry in both collection and processing. Once a large volume of low-cost polymer is available, scaling up and operating the process to yield desirable products with the required economies is difficult and costly. Viable polymer recycling plants have not been sufficiently demonstrated for most heterogeneous streams.

Chemical Manipulations

Once a mixed polymer stream is available, the highest-priority barrier is the lack of understanding of the chemistry and processes that are needed to cost-effectively depolymerize the stream and make it compatible with other process requirements. Knowledge of chemistry is needed to modify polymers for new uses and to derive pure monomers. The ability to chemically manipulate streams is a limiting factor for product recovery, and determines which polymer streams are potential sources of a desired product (e.g., which will yield monomers for new polymers).

R&D Infrastructure

A critical barrier is the lack of R&D to address processing needs and to set standards for recycled polymers. Public-private partnerships are not always available to participate in the market or to field-test new approaches.

Markets

Many of the technical barriers address the cost-effectiveness of polymer recovery and processing for final use. Market barriers include the difficulty of obtaining sufficient supplies of the desired type of post-use materials, and identifying industries to purchase the recovered polymers and monomers. Market determinants include the price gap between recycled and virgin material, and the use of competitively priced polymers in new applications while meeting quality and reliability requirements.

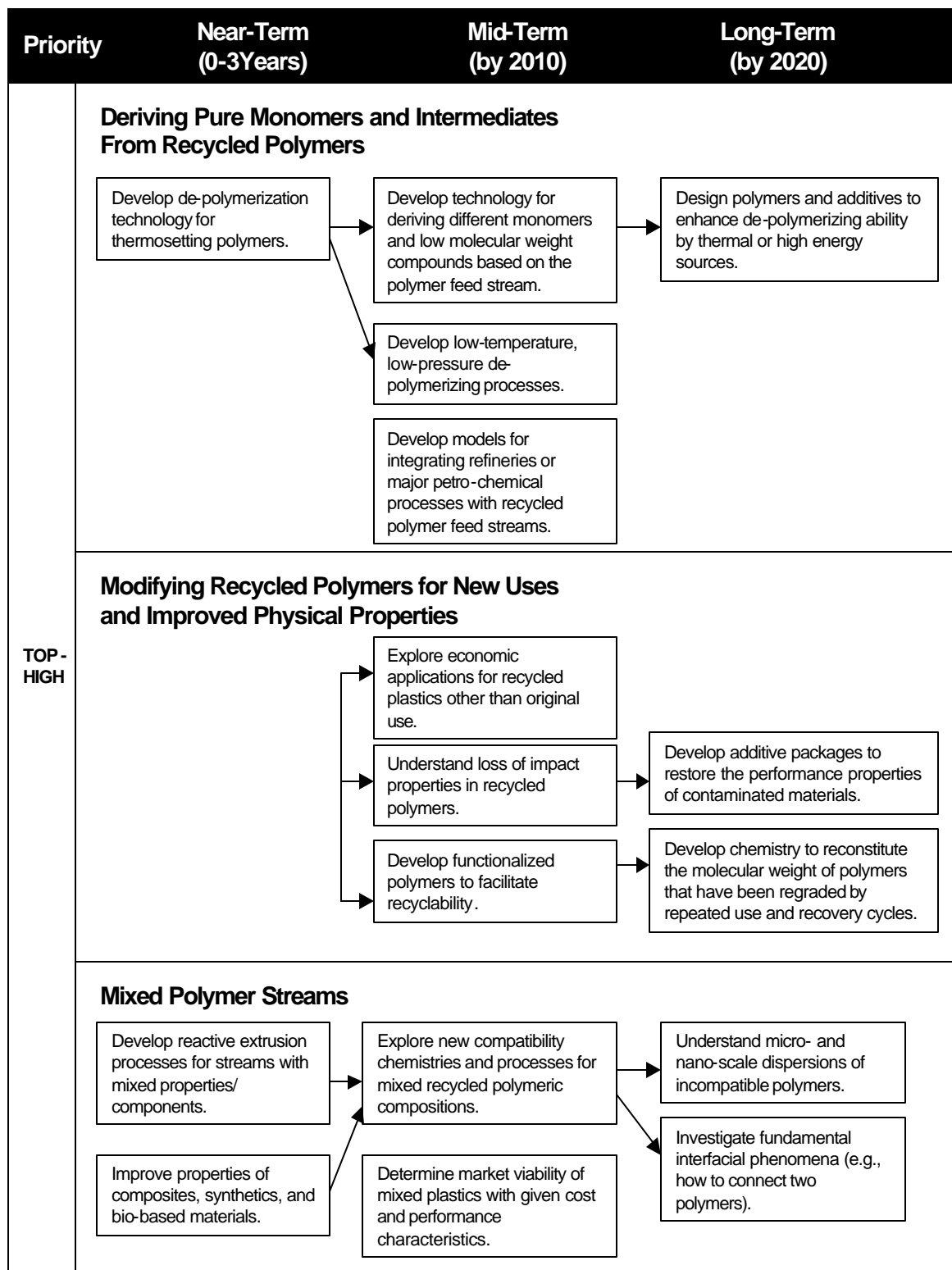
Policies and Structures

Polymer recycling has become its own industry, yet there is no one organization that is assisting manufacturers in learning how to recycle the post-use material, link material suppliers with recyclers, or identify the knowledge gaps in the recycling industry where R&D should be targeted. A significant barrier to polymer recycling is the lack of industry- or government-driven policies to establish a more effective market. For example, policies could standardize polymer composition in new product manufacturing in order to foster recovery, and set performance standards for polymers and monomers recovered from post-use materials.

High Priority Research Needs

The priority research and development needed to foster advances in disassembly, recovery, and recycling technology are illustrated in Figures 6-3, 6-4, and 6-5, including the timeframe in which

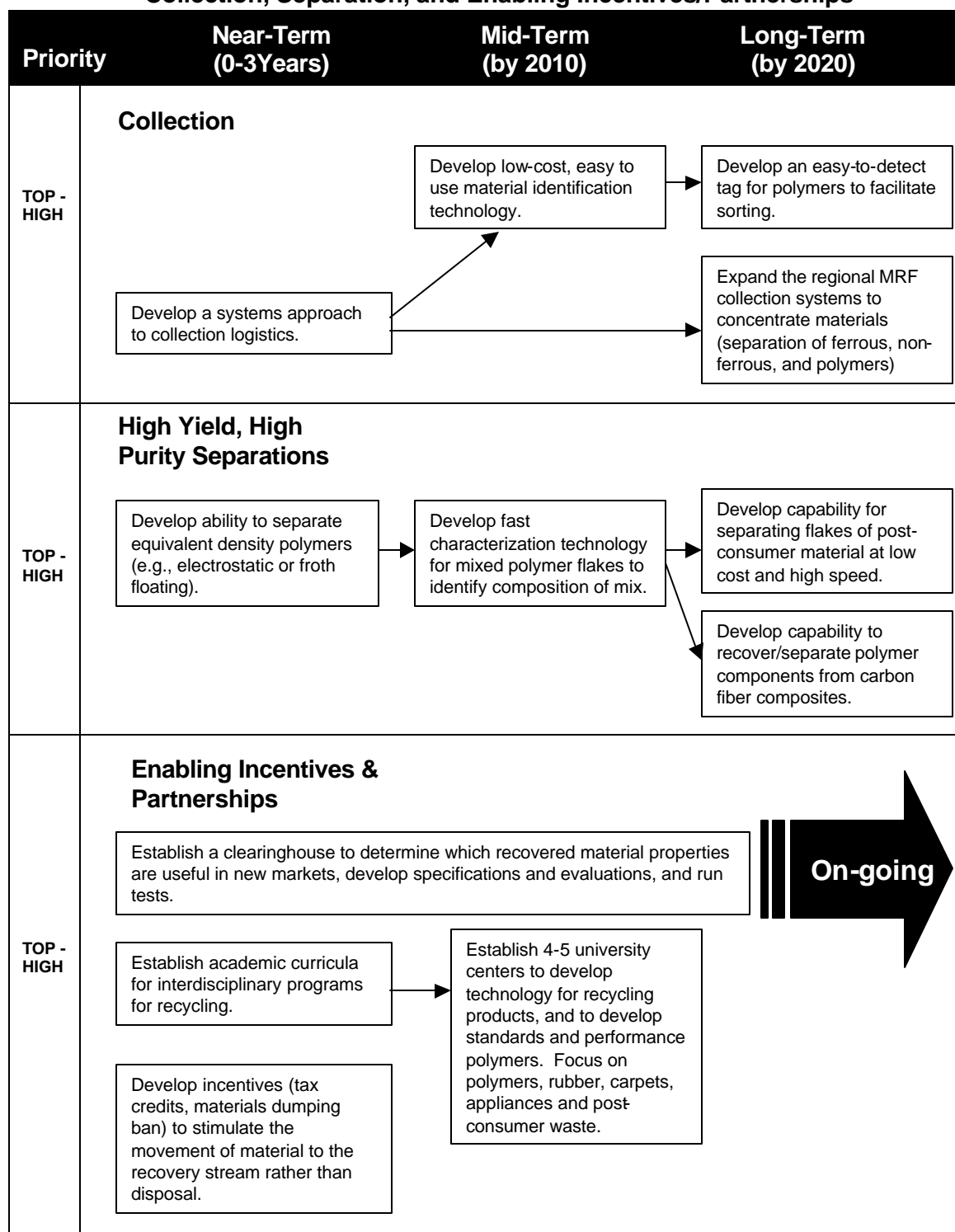
**Figure 6-3. R&D Needs for Disassembly, Recovery and Recycling:
Fundamental Science and Chemistry**



**Figure 6-4. R&D Needs for Disassembly, Recovery and Recycling:
Design for Recycling and Technology Demonstration**

Priority	Near-Term (0-3Years)	Mid-Term (by 2010)	Long-Term (by 2020)
TOP HIGH	Worldwide Design for Recycling		
		Promote technology to avoid irreversible contamination in product design (I.e., avoid painting, gluing, and melting).	<div>Simplify the number of polymers contained in products.</div> <div>Broaden the core of polymers in more applications in order to rationalize the number of polymers.</div>
	Technology Demonstration		
	Demonstrate potential technology on appropriate scale to identify real costs and benefits (I.e.g, large sample sizes to determine recycling viability).		
	Clean Fuel Technology		
	Develop small-scale gasification technology.	Develop technology to recover heteroatom pollutants.	Develop cost-effective, non-polluting combustion technology to burn polymers cheaply and cleanly.

**Figure 6-5. R&D Needs for Disassembly, Recovery and Recycling:
Collection, Separation, and Enabling Incentives/Partnerships**



meaningful results and process improvements can be expected from the research. A complete table of R&D needs in this area is provided in Appendix B.

Easy, Low-Cost Accessible Ways To Collect Raw Materials

R&D related to further collection of post-use material falls into two categories: incentives and logistics, and technology-sorting capabilities. Incentives are needed to motivate end-users to concentrate materials and send them into the recovery stream. The collection process needs to become more efficient through systems logistics. Sorting technology is needed to identify the types of polymers in a material and determine whether it is more cost-effective to sort at the collection site, at an intermediate location, or at the processing facility. To facilitate collection and recycling, a useful coding system to identify polymer content in products needs to be developed and adopted industry-wide. Eventually, polymer “tags” would help facilitate sorting.

Chemistry Processes for Mixed Polymer Streams

High-priority needs in this category are to improve properties of composites, synthetics, and biobased-materials, and to develop functionalized polymers to facilitate recyclability. Another research need is to develop technology and processes to restore impact properties and other characteristics that are degraded in recycled polymers. Research is also needed to understand the chemistry of micro- and nano-scale dispersions of incompatible polymers.

Deriving Pure Monomers and Intermediates from Polymers

The highest-priority research need in this category is developing technology to isolate pure monomers from mixed polymers. Another priority research need is the development of models for integrating petrochemical processes with polymer recycling. Developing the capability to depolymerize at low temperature and pressure is a research need and includes depolymerizing thermosets. In addition, research is needed to develop catalytic routes to higher selectivity.

Chemistry To Modify Polymers for New Uses and Chemistry of Physical Properties

The highest-priority research need in this category is to develop compatible chemistries and processes for mixed polymers including the capability to evaluate cost and performance for a given sample. Technology and processes are needed to restore the polymeric performance of contaminated material. Another priority research need is the development of reactive extrusion processes for mixed polymers, and understanding fundamental interface phenomena to connect two polymers. Developing technologies to remove contaminants such as paint, dyes, and adhesives are also needed. An on-going research effort is to needed investigate uses for recovered polymers.

High-Yield, High-Purity Separation Processes

The highest-priority R&D need identified for materials and techniques for recycling is the development of technology and processes to separate equivalent-density polymers. Developing technology to sort and separate polymer flakes is an important industry priority. Technology is also needed to quickly identify the polymers in a sample of mixed polymer flakes. As the sample mix is evaluated, technology is needed to separate the flakes at low cost and high speed. Other needs in separations research include using supercritical carbon dioxide for impurity removal, and developing methods to remove paper from polymer streams and to recover polymers from carbon fiber composites. On an ongoing basis, research is needed to evaluate the cost-effectiveness of polymer collection and sorting.

Economically Viable Polymer Recycling for Large-Volume, Low-Cost Polymers

Demonstrations are needed to investigate material recycling processes. The highest-priority R&D need is to demonstrate technology in large enough sample sizes to provide real-world cost

estimates and explore the impact of new technology and processes. Another need is to determine what is a statistically relevant sample size to evaluate material recovery streams for down-stream processing.

Focused R&D To Assist Recyclers

(Public-Private Partnerships To Test and Set Standards)

Research and industry should be organized to promote polymer recycling. The highest-priority research needs are determining performance specifications for new markets through testing, developing process technology for polymer identification and separation, and distributing useful information through a clearinghouse. It is essential to determine what is known about polymer recycling and identify the knowledge gaps. Collaboration is needed among industry, universities, and laboratories to promote economically viable process technology and industry development. Interdisciplinary education is also needed.

Design for Recycling Worldwide

Incorporating specifications for recycling in product design and development could improve the supply and cost-effectiveness of materials in the future. R&D is needed to develop “design for recovery” strategies that can be used throughout the manufacturing industry, such as simplifying the number of polymers in any one application and throughout the manufacturing industry. Design strategies are also needed to reduce contamination of the supply stream from paints and glues, and facilitate the ease of disassembly during collection and sorting.

Clean Fuel Technology

To foster the use of polymers as an energy source (where appropriate and cost-effective), research is needed to develop clean combustion through fuel processing or recovering the by-products of combustion, such as hetero-atom recovery. The highest-priority R&D need is the development of small-scale gasification technology for diverse applications.

Appendix A: Workshop Participants

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Appendix B
Detailed Tables
Research & Development Needs for
Material Technology

Exhibit B-1. R&D Needs for New Materials (includes both workshops)
 (☼ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Prediction/ Simulation Characterization	Fundamental Science	Polymer Chemistry	Process/ Design/ Engineering	Specialty Materials/ Biomaterials	Lifetime Prediction Analysis
NEAR (0-3 Years)		Research to synthesize/develop new nanoparticle platelets F	Develop one-pot cross- linking technology at ambient conditions (no heating) S new cross linking chemistry		Organic materials with improved fire resistance MMMMF	
		R&D on compatible blends of materials F	S coating systems based on customer need		Develop reaction-injection moldable molecular composites CMF	
		Polymer additives to improve paper products and paper making S reduce amount of pulp used	S obviates need for mixing before applying		Explore anti-fouling, anti- graffiti coatings Explore better concepts for compatibility that give readily process-able blends ☼☼	
			Conduct more R&D on monomerization for condensation polymers		Develop polymer blends and grow the market MM	
					Develop thermo sets with thermopolymer properties MM	
					Develop "one-pot" thermosetting systems for coatings and adhesives M	
					Develop new adhesives for underwater applications (e.g., barnacle type)	

Exhibit B-1. R&D Needs for New Materials (includes both workshops)
(☺ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Prediction/ Simulation/ Characterization	Fundamental Science	Polymer Chemistry	Process/ Design/ Engineering	Specialty Materials/Biomaterials	Lifetime Prediction Analysis
MID (3-10 Years)	<p>Examine tribology and wear in polymers, rubbers, and other materials ☺☺☺M</p> <p>Develop computational methods for catalyst design ☺MMMMF</p> <p>Develop better methods of characterizing composites during fabrication ☺MF</p> <p>Improve the ability to design/predict interaction between polymers</p> <ul style="list-style-type: none"> – miscibility control at interface – multi-component (>3) ☺ <p>Apply combinatorial chemistry to understand/predict catalytic structure and property activity M</p>	<p>Explore mechanisms governing equations for structure-property relationships ☺MMMF</p> <p>Improve molecular structure control in free radical polymerization (e.g., PAN, PMMA, PVC, PS) ☺MMM</p> <p>Synthesis of inorganic/ organic hybrids ☺☺FF</p> <p>Develop scientific basis for fabrication and optimization of hybrid composites ☺FF</p> <p>Explore structure, chemistry, and properties of natural systems (e.g., spider webs) MM</p> <p>Improve methodologies for articulating nano - scale topography on surfaces M</p> <p>Develop high compressive strength around fibers M</p> <p>Develop artificial ribosome - template for ordering F</p> <p>New compatible reaction chemistries F</p> <p>Explore thermally reversible cross links (e.g., in rubbers) F</p> <p>Use polymers to eliminate flaws in traditional materials (paper, glass) S study interaction between polymers and traditional materials</p> <p>Explore ways to speed up reactions in bioprocess</p> <p>Explore interfacial reactions between polymer and fiber polymers/metals, etc., including mechanics and physics</p>	<p>R&D on C1 chemistry applied to monomers ☺☺☺MF</p> <p>Explore new ethylene and polar-functional monomers MMF</p> <p>S entirely new families of materials</p> <p>Develop early phase modeling of catalysts for polymeric systems M</p> <p>Develop cost-effective living free-radical polymerization processes for large scale applications F</p> <p>Catalyst research related to CO₂ addition reactions F</p>	<p>Develop alternate processing methods (fibers, films) MMF</p> <p>Develop catalytic processes that work in water MF</p> <p>Develop methods of utilizing molecular orientation to get molecular strength in more than one direction</p> <p>Conduct R&D on control and stability of dimensions and shape at the macroscopic level</p> <p>Explore techniques for environmentally friendly film formation</p>	<p>High temperature proton exchange membrane (PEM) materials for fuel cells) (120-150°C) ☺MMF</p> <p>New materials for more selective separation (high permeability and thermal stability) MMF F</p> <p>Explore molecular concepts for more effective barrier materials for packaging foods, pest control (e.g., oxygen, CO₂, H₂O) ☺M</p> <p>Conduct coatings research to improve MF F</p> <p>S properties of materials, corrosion mollusks/micro-organisms</p> <p>S surface chemistry</p> <p>Develop carbon-based materials MF</p> <p>S nanoscale control of porosity</p> <p>S low-cost carbon fiber</p> <p>S polymer precursors for molecular sieves</p> <p>R&D to increase use of polymers in novel agricultural projects MF</p> <p>Explore low-cost, two- dimensional reinforcement fillers M</p> <p>Explore new polymer solvents to replace organic solvents M</p> <p>Develop high-filled (80+%) polymeric composites designed for specific application F</p> <p>Develop dendritic polymerization-controlled structural materials F</p> <p>Robust chemical modification of polyolefin surfaces to get desired properties</p> <p>Exploratory study of higher-temperature polymers</p> <p>Identify new generations of polymers that are simultaneously reinforced (glass fiber and reinforced toughened rubber)</p>	

Exhibit B-1. R&D Needs for New Materials (includes both workshops)
(☼ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Prediction/ Simulation Characterization	Fundamental Science	Polymer Chemistry	Process/ Design/ Engineering	Specialty Materials/Biomaterials	Lifetime Prediction Analysis
LONG (>10 Years)	Conduct basic R&D to determine accurate guidelines for parameterization	<p>Explore mechanisms and develop governing evaluations for structure-property relationships ☼☼MMF</p> <p>Understand thin film adhesion and bonded interfaces (silicon, dispersed platinum-carbon copper) ☼MF</p> <p>S some fuel cell applications (platinum-carbon black)</p> <p>Apply combinatorial technology and methods to design, make and select polymers F</p> <p>Explore structure, chemistry, and properties of natural systems (e.g., spider webs) MM</p> <p>Develop high compressive strength around fibers M</p> <p>Develop artificial ribosome-template for ordering F</p> <p>Explore thermally reversible cross links (e.g., in rubbers) F</p> <p>Explore ways to speed up reactions in bioprocess</p>	<p>Explore brand new concepts in catalysis for polymers ☼☼☼F</p> <p>Find new materials through new synthetic processes (e.g. using monomers not used today, under different conditions) ☼☼FFF</p>	<p>Develop manufacture and fabrication processes that enable manipulation of structure at molecular levels ☼☼</p> <p>Research process modeling for new polymers S</p> <p>new processes S</p> <p>modify existing processes</p> <p>Develop structural materials S</p> <p>cold forming techniques applied to polymers S</p> <p>processing R&D</p>	<p>Characteriz/explore synthesis of inorganic/organic hybrids MMMMF F F</p> <p>Develop permeation - selective materials MMMMF</p> <p>Explore new fibers for carpet/home furnishings ☼F</p> <p>Develop new cost-effective forming/processing techniques MM</p> <p>Develop low coefficient thermal expansion (CTE) for isotropic films ☼</p> <p>Develop/explore materials for high temperature separations (300°C) ☼</p> <p>Conduct outside-the-box research to emulate desirable properties of natural fibers M</p> <p>Develop light-harvesting polymers or other materials F</p> <p>Explore metal-polymer hybrids (magnetic applications)</p> <p>Develop new materials for extremely high density information storage</p> <p>Conduct R&D to increase viability of inherently conducting polymers</p>	

Exhibit B-1. R&D Needs for New Materials (includes both workshops)
(☉ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Prediction/ Simulation Characterization	Fundamental Science	Polymer Chemistry	Process/ Design/ Engineering	Specialty Materials/ Biomaterials	Lifetime Prediction Analysis
ONGOING (Years)	Conduct research to bridge gap between scales S understanding structures S molecular dynamics and continuum mechanics S determining which scales are important for specific designs ☉☉☉☉☉☉☉ Develop computational tools for prediction and design of polymeric materials ☉MM	Study of polymer structure-property relationships including fabrication structure-property relationships at the microstructure level ☉MMMF Colloid science ☉☉☉☉F S extending new colloids and science to polymers S tremendous growth as result of ceramic science S new tools and science available Models and data for life-time prediction MF S degradation mechanisms Greater control of supermolecular assemblies M S understand intermolecular interaction for design/control of structural function	Develop better recycle schemes for polymers ☉ S catalysts to depolymerize S mass transport schemes S broad range of R&D Thermally reversible polymer materials		Make new monomers MMF Develop polymeric materials from renewable sources M Develop biodegradable, cheap polymers with improved properties F Conduct more targeted materials research (i.e., replace specific type of material) S R&D in a team environment with industry, marketing, faculty, etc. Develop polymers for in-line sensors S temperature S olfactory Develop materials for computer technology	Develop more sensitive techniques to detect aging in real-time models, including methods that integrate chemical, mechanical, and thermal effects ☉☉☉☉☉MF Develop tools to diagnose and screen the state of a material to determine aging mechanisms ☉F Explore mechanisms of environmental stress cracking in polymeric materials ☉ Explore mechanisms of thermal and environmental degradation in polymers M Model/predict behavior of (glass reinforced) phenolic and epoxies composites in aggressive and corrosive environments

Exhibit B-1. R&D Needs for New Materials (includes both workshops)
 (★ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Prediction/ Simulation Characterization	Fundamental Science	Polymer Chemistry	Process/ Design/ Engineering	Specialty Materials/Biomaterials	Lifetime Prediction Analysis
ONGOING (Years)	<ul style="list-style-type: none"> take atomistic models and predict morphologic effects sequence control/molecular recognition 	Research to improve materials processing conditions M <ul style="list-style-type: none"> less energy and emissions eliminate VOC's lower temperature lower costs 				
	Develop analytical techniques for characterizing materials behavior <ul style="list-style-type: none"> S tests S diagnostics S usable database ★MMFF 	Make existing polymers/monomers cheaper M Explore economical ways to exploit break-through in polymer architectures Understand properties in thin films at the molecular level				
	Conduct exploratory R&D and assessments to match market needs to new materials F					

Exhibit: B-2. R&D Needed for Materials Characterization (⚡ = Top Priority; M = High Priority; F = Medium Priority)				
Time Frame	R&D Tools	Real-Time	Modeling & Stimulation	R&D Education
NEAR (0-3 Years)	Carry out R&D to determine endpoint of reaction F	Measure <ul style="list-style-type: none"> – composition – elongation 		Stress oral & written communication
	Conduct materials characterization in addition to chemical characterization ⚡OMF Develop inert labeling or non-labeling techniques for imaging interfaces MMF	Develop molecular-level embedded sensors MMFF <ul style="list-style-type: none"> – robust sensor packaging for harsh environments 		
NEAR - MID (Years)				
MID (3-10 Years)	Use high-throughput assay methods for generation of database <ul style="list-style-type: none"> – high data throughput detectors ⚡⚡⚡MMMF Conduct R&D in how thin films are influenced by other materials <ul style="list-style-type: none"> – confined geometries ⚡M Carry out R&D in ultrasonic processes M Develop advances in spectroscopy to obtain more detailed macro - molecular information F Use time-resolved spectroscopy	Study <ul style="list-style-type: none"> – real-time rheological measurements – need for real-time data compression and manipulation – closed-loop control 		Gain exposure to collaborative interdisciplinary research <ul style="list-style-type: none"> – requirements for Ph.D. in chemistry or engineering should be diversified – students should be “well-read” ⚡⚡⚡⚡MMM Examine the language and approaches used in life sciences MMMF Incorporate interdisciplinary cross-over F Have a total systems approach as to how a material is made and used
MID - LONG (Years)	Develop separation in/or discrimination methods ⚡M Expand characterization techniques used at the micro-structure	Develop buried sensors that measure methodology properties <ul style="list-style-type: none"> – acoustics micro sensors 		

Exhibit: B-2. R&D Needed for Materials Characterization (⚡ = Top Priority; M = High Priority; F = Medium Priority)				
Time Frame	R&D Tools	Real-Time	Modeling & Stimulation	R&D Education
	level F Carry out R&D to change the speed of measurement by at least two orders of magnitude F			
LONG (>10 Years)	Develop new techniques for composition, structure, and dynamics for buried interfaces – 3-dimensional imaging – chemical information imaging – mechanical imaging ⚡⚡⚡MMMMF F Conduct R&D in aging *also modeling issue ⚡⚡F Mine data for the generation of knowledge (infometrics) ⚡M Develop method of sequencing complex mixtures MMM Study the need to characterize the dynamic structure of materials *also modeling M Work out better methods for analyzing complex polymers (copolymers, amorphous, and others) FFF Make imaging techniques direct	Make on-line measurements for non-experts – spatially resolved, non-contact ⚡⚡⚡⚡⚡FF Use real -time, non-destructive, online monitoring & control of materials processing ⚡⚡MF	Prepare models on molecular level and on performance level (simulation) – semi-empirical models – 1 st principle models – massively parallel computations ⚡⚡MMMMMMMF F Devise methods to predict material properties from polymer structure – primary, secondary, tertiary structure MMMF	

Exhibit B-3. R&D Needs for Modeling
 (⊕ = Top Priority; M = High Priority; F = Medium Priority)

R&D Area	R&D Time Frame		
	Near Term (0-3 years)	Mid Term (3-10 years)	Long Term (>10 years)
Methods Development	<p>Develop accurate potentials ⊕⊕⊕⊕⊕F</p> <p>Develop methods at the mesoscale ⊕MMMFFF</p> <p>Develop hybrid and quantum techniques ⊕F</p> <p>Efforts in parallel algorithms and implementation MMF S smart algorithms</p> <p>Establish a general consensus on different classes of mesoscale models MF</p> <p>Implement new mathematical techniques for molecular modeling M S multi-grid/multi-scale</p> <p>Further extend open ensemble simulation techniques (ambient temperature)</p>	<p>Develop algorithms for including chemical reactions in supra-electronic structure simulations M</p> <p>Develop new methods for predicting and characterizing self assembly and mechanical properties in biological systems FF</p> <p>Develop ways to mimic the environment that are better than periodic boundary conditions S general solutions</p> <p>Develop improved free energy/chemical potential methods</p>	
	<p>Multi-faceted, multi-disciplinary, coordinated theory/modeling/experimental research effort in interfaces ⊕⊕MMFFFF</p> <p>S aqueous systems</p> <p>S polymer liquid crystal-line interfaces</p> <p>S polymer interface with inorganic solids</p> <p>S multi-phase</p> <p>S multi-component</p> <p>S dissimilar surfaces</p> <p>S bio-materials</p> <p>S filled polymers and nano-composites</p> <p>Explore new methods to model newly developed materials</p>		

Exhibit B-3. R&D Needs for Modeling
(⊕ = Top Priority; M = High Priority; F = Medium Priority)

R&D Area	R&D Time Frame		
	Near Term (0-3 years)	Mid Term (3-10 years)	Long Term (>10 years)
Theory	Encourage development of basic theory for materials science ⊕⊕M Support R&D on solvation models	Better understand connection between lab-scale properties and performance M Understand electrical conductivity of bulk band gap materials	Develop integrated models that combine chemistry and physics in complex multi-phase systems
	Improve bridging techniques ⊕⊕⊕⊕⊕MMF S revisit renormalization group approach as bridging link S encourage academic research on bridging length and time scales S mapping and reverse mapping Develop better theories and modeling methodology for non-equilibrium conditions (e.g., aging) ⊕FFF Explore how processing affects ultimate properties ⊕ S processing makes micro-structure, which determines ultimate properties S increase fundamental knowledge		
Organizational	Conduct validation in a systematic way using benchmarks and standards ⊕MMFFFF Implement best practice in research partnership (European Framework Five may be a good example) S public validation of deliverables Develop data and tools to validate simulation tools	Explore new business process R&D to overcome organization and process issues	
Materials			Model poorly defined materials that are important to industry MMM S e.g., carbon black, halt
Model crystal formation in semi-crystalline polymers MMF			
Hardware/ Software		Understand how to use parallel PCs FF Improve problem-solving environments	Explore better ways of interacting with computers (human-computer interaction) S voice recognition (VR) S artificial intelligence S complex systems S VR environments
	Develop software that makes the most effective use of existing and new hardware F		

Exhibit B-3. R&D Needs for Modeling
 (⚙ = Top Priority; M = High Priority; F = Medium Priority)

R&D Area	R&D Time Frame		
	Near Term (0-3 years)	Mid Term (3-10 years)	Long Term (>10 years)
Enabling Tools	<p>Develop tools for deriving accurate quantum chemistry-based atomistic potential simulations</p> <p>Improve information dissemination</p> <p>S web-based information communication - communicate to community</p> <p>S distribution lists for modeling</p>	<p>Improve data mining and discovery tools ⚙MF</p> <p>S interact with data in a useful way</p> <p>Establish a central, publicly accessible repository of data and validation tools M</p> <p>Develop standards for data structures, data input/output and interfaces F</p> <p>Establish a database for computational results and quality measures</p>	
Education	<p>Integrate modeling and simulation techniques into undergraduate and graduate curricula MM</p> <p>Publicize success stories in short form (for management education)</p> <p>S which company</p> <p>S what result MFF</p> <p>Implement an engineering course in chemistry PhD programs F</p> <p>Establish QSAR, QSPR techniques for academia</p> <p>Academic research projects should use modeling in their work (Master's, PhDs)</p> <p>Encourage universities to implement more training in modeling and scientific method</p>		

Exhibit B-3. R&D Needs for Modeling
(☉ = Top Priority; M = High Priority; F = Medium Priority)

R&D Area	R&D Time Frame		
	Near Term (0-3 years)	Mid Term (3-10 years)	Long Term (>10 years)
Cultural	<p>Find a mechanism for jointly defining industrial problems for academic research ☉</p> <p>Encourage development of more, better, reliable, robust, portable and extensible simulation tools</p> <p>Encourage more “take a chance” funding</p> <p>Convince students that modeling is important and industry is interested in modeling</p>	<p>Multi-disciplinary, multi-institutional teams need incentives to undertake R&D S funding and tenure systems S e.g., fundamental particle physics</p>	
Implementation and Integration	<p>Encourage development of templates for integration of data and models into product/process development ☉M</p> <p>Reduce results of molecular modeling to a design heuristic M S users see a design rule</p> <p>Present results of models in QSAR, QSPR to technology users M</p> <p>Combine materials modeling with optimization under presence of uncertainty F</p> <p>Apply well-developed techniques from computational biology to self assembly F</p>	<p>Broaden the use of modeling by making methods more easily accessible F</p>	<p>Use molecular models in real time for process control where appropriate</p> <p>Integrate modeling and artificial intelligence</p>

Exhibit B-4. Priority R&D Needs for Additives Development
(Top Priority; *Priority*)

Time Frame	Multi-purpose Additives	Property Modification	Advanced Processes	New Flame Retardant Additives	Bio-compatible & Bioactive	Stabilization & Control	Structure Property Relationships	Characterization Methods	Cooperation
NEAR (0-3 Years)			Develop new synthetic routes for "green" additives and environmentally friendly properties to lower emissions of VOCs						Explore efficiency of industry-university partnerships in research
MID (3-5 Years)		Develop nano particle fillers with more interface area to lead to increased effectiveness Develop and understand additives that can lead to polymers with previously unseen balance, toughness, stiffness (i.e., high modulus and high fracture toughness Anti-static control without optical, coloring or environmental	Develop means of reducing particle size to submicron levels with narrow particle size distribution (e.g., 0.5 micron)	Develop non-halogen vapor-phase flame poison	Develop biobased and recyclable polymers for packaging applications	Develop antioxidant chemistry that can be catalytic rather than sacrificial	Develop understanding of the surface chemistry of additive interfacial interactions	Develop experimental methods to explore interfacial regions Develop more sensitive analytical techniques for trace analysis	

Exhibit B-4. Priority R&D Needs for Additives Development
(Top Priority; Priority)

Time Frame	Multi-purpose Additives	Property Modification	Advanced Processes	New Flame Retardant Additives	Bio-compatible & Bioactive	Stabilization & Control	Structure Property Relationships	Characterization Methods	Cooperation
LONG (> 10 Years)			Develop defect-free polymers				Develop seamless multi-scale portfolio of computational methods for additives and polymers for study and prediction of properties Develop models to handle multi-phase systems on a scale large enough to predict physical properties		
ON-GOING									Provide financial support for near-term needs of additives R&D M

Exhibit B-5. R&D Needs in Additives
 (⊕ = Top Priority; M = High Priority; F = Priority)

Structure Property Relationship		Characterization Methods	Cooperation Between Industry, Academia, and Government (pre-competitive)	Advanced Processes
Predictive Modeling	Understand Performance Mechanisms			
Develop seamless multi-scale portfolio of computational methods for additives and polymers for study and prediction of properties ⊕⊕⊕⊕⊕⊕	Develop understanding of surface chemistry of additives (interfacial interactions) ⊕⊕⊕MM	Develop experimental methods to explore interfacial regions MMMFF	Develop realistic global environmental regulations MMF	Develop defect-free polymers MF
Develop modeling systems to handle multi-phase systems on a scale large enough to predict physical properties ⊕⊕	Develop better understanding of fracture mechanics, relating polymer properties to physical properties ⊕⊕⊕M	Develop more reliable accelerated aging techniques MM	Explore efficiency of industry-university partnerships in research and teaching M	Develop means of reducing particle size to submicron levels with narrow particle size distribution (e.g., 0.5 micron) FFFF
Develop better models for viscous fluid dynamics to develop better multi-phase models for melt processing	Generate advanced understanding of the function of additives ⊕	Develop more sensitive analytical techniques for trace analysis M	Provide financial support for near-term needs of additives R&D M	Develop new synthetic routes for “green” additives and environmentally friendly properties to lower VOCs M
Develop performance modeling to anticipate new materials needs	Explore properties of nano-fillers F	Develop, measure and control non-equilibrium processing F	Develop consortia for multi-scale modeling F	Develop safe materials handling for any new organic additive (consider explosivity and worker exposure)
	Develop full understanding of rigid particle toughening	Develop high-thru put combinatorial methods for material science	Develop better incentives to encourage industry to enter into joint ventures with academia F	Develop filler-polymer blending technology suitable for e-commerce
	Develop better understanding of degradation mechanisms of commercial polymers	Develop rapid analytical methods to study interfacial chemistry (e.g. additive effectiveness)	Sponsor high profile individual to educate the public about what additives contribute (benefits)	Develop new reactor additives to add during polymerization
	Develop understanding of the role of solubility and diffusion for effectiveness of stabilizers and antioxidants		Expedite new product development without getting caught up in process and business models (e.g., identify properties and then translate to benefits)	Develop methods to introduce additives into transgenic synthesis of polymers (e.g. move an antioxidant into polymer that is grown transgenically)
	Understand impacts of impurities (e.g. for proper separation)		Establish polymer additives consortium	Develop real time process measurement and control
	Develop the capability to engineer thermopolymers with a “continuous use temperature” >200°C		Provide tax breaks for industry to sponsor and mentor high school and university students in relevant technical areas	Develop cost effective particle dispersion

Exhibit B-5. R&D Needs in Additives
 (☉ = Top Priority; M = High Priority; F = Priority) (continued)

New Additives					
Property Modification		Flame Retardant	Stabilization & Control	Bio-compatible & Bioactive	Multi-purpose Additives
Nanoparticle fillers— more interface area to increase effectiveness ☉☉FF	Develop property enhancers at low addition levels F	Develop non-halogen vapor phase flame poison ☉	Develop antioxidant chemistry that can be catalytic rather than sacrificial ☉☉	Develop bio-compatible polymers and additives MM	Develop multi-functional additives ☉MF
Develop fillers with improved capability to control polymer morphology MM	Develop cost-effective melt processing aids that do not react with other additives F	Develop catalytic flame retardant agents ☉	Develop thermal stabilizers effective at > 250°C FF	Develop biobased and recyclable polymers for packaging applications ☉	Develop additives to sense and communicate (e.g., change color) FFFF
Develop and understand additives that can lead to polymers with previously unseen balance, toughness, stiffness (i.e., high modulus and high fracture toughness) MF	Develop new anti-static additives for high temperature application >250°C (e.g., 10,000 hours) F	Develop new flame retardants that give rise to low smoke and heat release (e.g. nano-composites) FF	Develop ultraviolet absorbers with at least double the photostability of present materials FF	Develop broad range of fillers for biopolymeric applications (i.e., bio-compatible, bio-active) F	Functional stabilizers via a speciality co-monomer F
Anti-static control without optical, coloring, or environmental effects	“Develop adjustable properties” through additive concentration to enable recyclability	Develop self-extinguishing thermopolymers	Develop UV absorbers with double the absorptivity F	Develop additives for biodegradable polymers	Explore multi-functional additives (e.g. electrical conductivity, applications other than color, crystal)
Develop stable, light-fast, non-toxic colorants (i.e., pigments and dyes) M		Develop additives that shift and/or respond to “light” and/or “energy” besides ultraviolet (UV)	Develop additives to control the lifetime of components and polymers	Explore the use of natural stabilizers (e.g. vitamin E)	Develop self regulating and controlled release fillers
Develop impact modifiers that can be processed at greater than >300°C and be effective at	Explore new methods for functionalizing filler surfaces to engineer new properties in composites		Develop high temperature stabilizers for 300 to 400°C melt processing/fabrication	Develop biologically active additives for disease control and biological protection	Develop additives that can indicate physical phenomena (i.e., oxidative, chemical, electrical)
			Develop additives that enable controlled biodegradation of polymers	Develop completely biodegradable polymer system without any environmentally unfavorable consequence	

Exhibit B-5. R&D Needs in Additives
 (⊕ = Top Priority; M = High Priority; F = Priority) (continued)

New Additives					
Property Modification		Flame Retardant	Stabilization & Control	Bio-compatible & Bioactive	Multi-purpose Additives
–50°C F	Develop impact modifiers or tougheners for thermoset composites that can be resin-transferred (e.g. for infrastructure uses)		Develop new additives to control and/or deactivate structural defects in polymers Control and/or deactivate impurities in the polymer system	s (i.e. low toxicity)	
Explore creation of new additives/fillers with controlled morphology, surface chemistries, and functionality F	Develop transparent polymers with a 10 fold reduction in permeability via additives (e.g., H ₂ O, O ₂ , CO ₂ , etc.)				
Develop new conductive polymers or fillers for lower addition-levels in polymers F					

Exhibit B-6. R&D Needs for Disassembly, Recovery, Recycle, Reuse and Renewable Technology
(☼ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Easy, Low-Cost Accessible Way to Collect Raw Material	Understanding Chemistry Processes for Mixed Polymer Streams	Understanding How to Derive Pure Monomers and Intermediates from Polymers	Understanding Chemistry to Modify Polymers for New Uses and Chemistry of Physical Properties	High-Yield, High-Purity Separation Processes	Demonstrate Economically-Viable Plastic Recycling for Large-Volume Low-Cost Polymers	Focused R&D to Assist Recyclers (Public-Private Partnership s to Test and Set Standards)	Design for Recycling Worldwide	Clean Fuel Technology
NEAR (0-3 Years)	Develop incentive approaches to stimulate the movement of material to a recovery stream -- not to the dump (e.g., tax credits and material ban at dump) ☼MF F	Improve properties of composites, synthetics and bio-based material F F F Develop stabilizers and antioxidants to prevent degradation of polymers	Develop depolymerization for thermosets F	Develop reactive extrusion processes for mixed property streams ☼MF Develop technology to remove paints and adhesives from waste polymers	Develop method for dealing with paper contamination in plastic Develop ability to separate equivalent density plastics (e.g., electrostatic or froth floating) ☼☼☼☼ F Explore supercritical CO ₂ for separation and removal of impurities	Demonstrate potential technology on appropriate scale to identify real costs (large sample sizes are needed to determine recycling viability) ☼MF Determine how big a demonstration is required Develop pilot for large scale demonstration of large volume polymers Investigate statistically appropriate sampling methods for material recovery streams	Establish a Gordin research conference on polymer recycling M Develop specific academic curriculum to establish interdisciplinary programs for recycling ☼		Develop small-scale gasification technology ☼☼
	Determine where along stream it is most cost efficient to separate and sort (if it is separable) Develop systems approach for collection logistics ☼☼ F								

Exhibit B-6. R&D Needs for Disassembly, Recovery, Recycle, Reuse and Renewable Technology
(♣ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Easy, Low-Cost Accessible Way to Collect Raw Material	Understanding Chemistry Processes for Mixed Polymer Streams	Understanding How to Derive Pure Monomers and Inter-mediate from Polymers	Understanding Chemistry to Modify Polymers for New Uses and Chemistry of Physical Properties	High-Yield, High-Purity Separation Processes	Demonstrate Economically-Viable Plastic Recycling for Large-Volume Low-Cost Polymers	Focused R&D to Assist Recyclers (Public-Private Partnerships to Test and Set Standards)	Design for Recycling Worldwide	Clean Fuel Technology
MID (3-10 Years)	Develop low-cost, easy-to-use identification technology FF Identify coding system for widespread use by manufacturers	Understand the loss of impact properties for recycled plastic M Determine combinations of material that are not easily sorted and develop processes for them Develop functionalized polymers to facilitate recyclability FF Develop understanding of technology for micro- and nano-scale dispersions of incompatible polymers M	Develop models for integrating refineries or major petro-chemical processes ♣♣F Develop processes to determine value of products produced (cost per lb) Develop low-temperature, low-pressure depolymerizing processes M Develop catalytic routes to higher selectivity M Develop technology for different monomers and low molecule weights based on the polymer feed stream ♣♣♣MMF	Determine what kinds of mixed plastic polymers could be market viable with a given cost performance characteristic ♣♣F Explore economic applications for recycled plastics (not original use) F Develop relevant impact test methods Develop new compatibility chemistries and processes for mixed recycled plastic compositions (cost versus performance-- properties need to be developed for each system) ♣♣MMF	Develop fast characterization technology for mixed plastic flakes to identify what is there ♣MMMF	Develop technology to recover hetero-atoms	Establish 4-5 university centers to develop technology to recycle products and develop standards and performance properties with a focus on plastics, rubber, carpets, appliances, and post-consumer waste -- Develop an internet-based hotline to answer questions-- Conduct research on performance versus costs of materials including market research on the relative magnitude of opportunities (e.g., how much polymer of what type is in a hair dryer) ♣♣M	Promote the avoidance of irreversible contamination in product design (i.e., avoid paint; glueing and melting) F	Develop methods to derive pure monomers Develop clean solid fuel from plastics Develop technology to recover hetero-atom pollutants F

Exhibit B-6. R&D Needs for Disassembly, Recovery, Recycle, Reuse and Renewable Technology
(☼ = Top Priority; M = High Priority; F = Medium Priority)

Time Frame	Easy, Low-Cost Accessible Way to Collect Raw Material	Understanding Chemistry Processes for Mixed Polymer Streams	Understanding How to Derive Pure Monomers and Intermediates from Polymers	Understanding Chemistry to Modify Polymers for New Uses and Chemistry of Physical Properties	High-Yield, High-Purity Separation Processes	Demonstrate Economically-Viable Plastic Recycling for Large-Volume Low-Cost Polymers	Focused R&D to Assist Recyclers (Public-Private Partnerships to Test and Set Standards)	Design for Recycling Worldwide	Clean Fuel Technology
LONG (>10 Years)	For longer-term, expand the regional MRF collection system to concentrate material (separate ferrous, non-ferrous and plastics) MFFF	Develop chemistry technology to reconstitute molecular weight of polymers that have been degraded by repeated use and recycling cycles F	Design polymers and additives to enhance depolymerizing ability by thermal or high energy sources Develop biotechnology-based depolymerization processes Develop better C-1 chemistry Develop selective oxidation reactions	Develop additive packages to restore performance properties of contaminant material ☼☼F	Develop ability to separate flakes of post-consumer material at low cost and high speed MMMMF			Simplify the number of polymers in products F Broaden the use of core plastics in more applications in order to rationalize the number of polymers FF	Demonstrate cost-effective, non-polluting combustion technology to burn plastics cleanly and acceptably
	Add an easy-to-detect tag to polymers to facilitate sorting F	Investigate the use of CO ₂ as raw material for polymeric composites F		Determine how to remove additives (e.g., dyes) Investigate high end uses for collected, recovered polymer materials	Develop measures of performance based on cost for plastic sorting and collection		Develop a clearinghouse to determine what properties are useful in new markets including developing specifications, evaluations, and running tests ☼MFFFF	Develop design and joining processes for dissimilar materials to enhance disassembly or recycling	Determine where it is appropriate and cost-effective to burn low-value material
ONGOING (All Periods)									

